# ESMValTool User's and Developer's Guide

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**ESMValTool Development Team** 

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# **ESMVALTOOL**

Ι	Introduction	1
1	About	3
2	Support	5
3	License	7
II	What ESMValTool can do for you	9
4	Data finding	13
5	Data selection	15
6	Data fixing	17
7	Variable derivation	19
8	Run the preprocessor	21
9	Run the diagnostics	23
III	Getting started	25
10	Installation	27
11	Configuration	39
12	Running	41
13	Output	43
IV	Gallery	47
V	Recipes	67
14	General-purpose diagnostics	71
15	Atmosphere	89

16 Climate metrics	211
17 Future projections	223
18 IPCC	305
19 Land	367
20 Ocean	405
21 Other	457
22 Broken recipe list	485
VI Obtaining input data	487
23 Models	491
24 Observations	493
25 Datasets in native format	499
VII Making a recipe or diagnostic	501
26 Introduction	503
27 Recipe	505
28 Diagnostic	507
29 Writing a CMORizer script for an additional dataset	509
VIII Contributing to the community	515
30 Contributing code and documentation	519
31 Making a new diagnostic or recipe	527
32 ESMValTool policy on backward compatibility	537
33 Broken recipe policy	541
34 Making a new dataset	543
35 Support for multiple versions of a dataset	547
36 Review of pull requests	549
37 Maintaining a recipe	553
38 Upgrading a namelist (recipe) or diagnostic to ESMValTool v2	555
39 GitHub Workflow	561
40 Moving work from the private to the public repository	567

41 R	elease strategy and procedure	569
IX	Utilities	583
42 Pı	re-commit	587
43 no	clcodestyle	589
44 C	olormap samples	591
45 R	unning multiple recipes	593
46 O	verview of recipe runs	597
47 C	omparing recipe runs	599
48 Te	esting recipe settings	601
49 dr	caft_release_notes.py	603
50 C	onverting Version 1 Namelists to Version 2 Recipes	605
51 R	ecipe filler	607
52 Ex	xtracting a list of input files from the provenance	609
XI	ESMValTool Code API Documentation	611
53 Sł	nared Diagnostic Code	615
54 Di	iagnostic Scripts	635
XI	Frequently Asked Questions	871
55 Is	there a mailing list?	873
56 W	/hat is YAML?	875
57 R	e-running diagnostics	877
58 Ei	nter interactive mode with iPython	879
59 Us	se multiple config-user.yml files	881
<b>60 C</b>	reate a symbolic link to the latest output directory	883
61 Ca	an ESMValTool plot arbitrary model output?	885
XII	Changelog	887
62 v2	2.10.0	889
63 v2	2.9.0	893

64 v2.8.0	897
65 v2.7.0	903
66 v2.6.0	907
67 v2.5.0	911
68 v2.4.0	915
69 v2.3.0	919
70 v2.2.0	923
71 v2.1.1	927
72 v2.1.0	929
73 v2.0.0	931
74 v2.0.0b4	935
XIII Indices and tables	937
Python Module Index	941
Index	943

# Part I

# Introduction

# ABOUT

The Earth System Model Evaluation Tool (ESMValTool) is a community-development that aims at improving diagnosing and understanding of the causes and effects of model biases and inter-model spread. The ESMValTool is open to both users and developers encouraging open exchange of diagnostic source code and evaluation results from the Coupled Model Intercomparison Project (CMIP) ensemble. This will facilitate and improve ESM evaluation beyond the state-of-the-art and aims at supporting the activities within CMIP and at individual modelling centers. We envisage running the ESMValTool routinely on the CMIP model output utilizing observations available through the Earth System Grid Federation (ESGF) in standard formats (obs4MIPs) or made available at ESGF nodes.

The goal is to develop a benchmarking and evaluation tool that produces well-established analyses as soon as model output from CMIP simulations becomes available, e.g., at one of the central repositories of the ESGF. This is realized through standard recipes that reproduce a certain set of diagnostics and performance metrics that have demonstrated its importance in benchmarking Earth System Models (ESMs) in a paper or assessment report, such as Chapter 9 of the Intergovernmental Panel on Climate Change (IPCC) Fifth Assessment Report (AR5) (Flato et al., 2013). The expectation is that in this way a routine and systematic evaluation of model results can be made more efficient, thereby enabling scientists to focus on developing more innovative methods of analysis rather than constantly having to "reinvent the wheel".

In parallel to standardization of model output, the ESGF also hosts observations for Model Intercomparison Projects (obs4MIPs) and reanalyses data (ana4MIPs). obs4MIPs provides open access data sets of satellite data that are comparable in terms of variables, temporal and spatial frequency, and periods to CMIP model output (Taylor et al., 2012). The ESMValTool utilizes these observations and reanalyses from ana4MIPs plus additionally available observations in order to evaluate the models performance. In many diagnostics and metrics, more than one observational data set or meteorological reanalysis is used to assess uncertainties in observations.

The main idea of the ESMValTool is to provide a broad suite of diagnostics which can be performed easily when new model simulations are run. The suite of diagnostics needs to be broad enough to reflect the diversity and complexity of Earth System Models, but must also be robust enough to be run routinely or semi-operationally. In order the address these challenging objectives the ESMValTool is conceived as a framework which allows community contributions to be bound into a coherent framework.

## SUPPORT

Support for ESMValTool can be found in ESMValTool Discussions page where users can open an issue and a member of the User Engagement Team of ESMValTool will reply as soon as possible. This is open for all general and technical questions on the ESMValTool: installation, application, development, or any other question or comment you may have.

## 2.1 User mailing list

Subscribe to the ESMValTool announcements mailing list esmvaltool@listserv.dfn.de to stay up to date about new releases, monthly online meetings, upcoming workshops, and trainings.

To subscribe, send an email to sympa@listserv.dfn.de with the following subject line:

• subscribe esmvaltool

or

• subscribe esmvaltool YOUR\_FIRSTNAME YOUR\_LASTNAME

The mailing list also has a public archive online.

## 2.2 Monthly meetings

We have monthly online meetings using zoom, anyone with an interest in the ESMValTool is welcome to join these meetings to connect with the community. These meetings are always announced in a discussion on the ESMValTool Community repository and on the *mailing-list*.

### 2.3 Core development team

- Deutsches Zentrum für Luft- und Raumfahrt (DLR), Institut für Physik der Atmosphäre, Germany (Co-PI)
  - ESMValTool Core Co-PI and Developer: contact for requests to use the ESMValTool and for collaboration with the development team, access to the PRIVATE GitHub repository.
- Met Office, United Kingdom (Co-PI)
- Alfred Wegener institute (AWI) Bremerhaven, Germany
- Barcelona Supercomputing Center (BSC), Spain
- Netherlands eScience Center (NLeSC), The Netherlands
- Ludwig Maximilian University of Munich, Germany

- Plymouth Marine Laboratory (PML), United Kingdom
- Swedish Meteorological and Hydrological Institute (SMHI), Sweden
- University of Bremen, Germany
- University of Reading, United Kingdom

## 2.4 Recipes and diagnostics

Contacts for specific diagnostic sets are the respective authors, as listed in the corresponding *recipe and diagnostic documentation* and in the source code.

#### THREE

### LICENSE

The ESMValTool is released under the Apache License, version 2.0. Citation of the ESMValTool paper ("Software Documentation Paper") is kindly requested upon use, alongside with the software DOI for ESMValTool (doi:10.5281/zenodo.3401363) and ESMValCore (doi:10.5281/zenodo.3387139) and version number:

Righi, M., Andela, B., Eyring, V., Lauer, A., Predoi, V., Schlund, M., Vegas-Regidor, J., Bock, L., Brötz, B., de Mora, L., Diblen, F., Dreyer, L., Drost, N., Earnshaw, P., Hassler, B., Koldunov, N., Little, B., Loosveldt Tomas, S., and Zimmermann, K.: Earth System Model Evaluation Tool (ESMValTool) v2.0 – technical overview, Geosci. Model Dev., 13, 1179–1199, https://doi.org/10.5194/gmd-13-1179-2020, 2020.

Besides the above citation, users are kindly asked to register any journal articles (or other scientific documents) that use the software at the ESMValTool webpage (http://www.esmvaltool.org/). Citing the Software Documentation Paper and registering your paper(s) will serve to document the scientific impact of the Software, which is of vital importance for securing future funding. You should consider this an obligation if you have taken advantage of the ESMValTool, which represents the end product of considerable effort by the development team.

# Part II

# What ESMValTool can do for you

The ESMValTool applies a great variety of standard diagnostics and metrics, and produces a collection of netCDF and graphical files (plots). Thus, the tool needs a certain amount of input from the user so that it can:

- establish the correct input and output parameters and the structured workflow;
- acquire the correct data;
- execute the workflow; and
- output the desired collective data and media.

To facilitate these four steps, the user has control over the tool via two main input files: the *user configuration file* and the recipe. The configuration file sets user and site-specific parameters (like input and output paths, desired output graphical formats, logging level, etc.), whereas the recipe file sets data, preprocessing and diagnostic-specific parameters (data parameters grouped in the datasets sections, preprocessing steps for various preprocessors sections, variables' parameters and diagnostic-specific instructions grouped in the diagnostics sections). The configuration file may be used for a very large number of runs with very minimal changes since most of the parameters it sets are recyclable; the recipe file can be used for a large number of applications, since it may include as many datasets, preprocessors and diagnostics sections as the user deems useful.

Once the user configuration files and the recipe are at hand, the user can start the tool. A schematic overview of the ESMValTool workflow is depicted in the figure below.

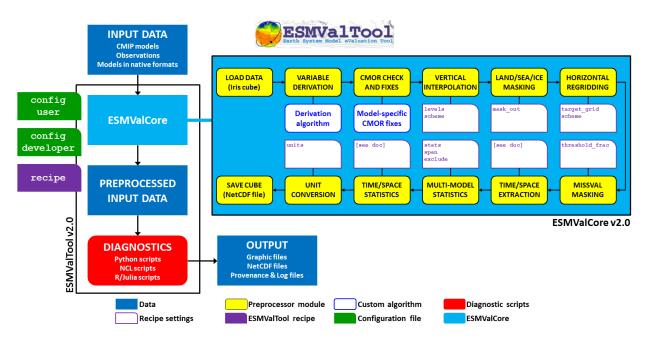


Fig. 1: Schematic of the system architecture.

For a generalized run scenario, the tool will perform the following ordered procedures.

## **DATA FINDING**

- read the data requirements from the datasets section of the recipe and assemble the data request to locate the data;
- find the data using the specified root paths and DRS types in the configuration file (note the flexibility allowed by the data finder);

## FIVE

## **DATA SELECTION**

• data selection is performed using the parameters specified in the datasets section (including e.g. type of experiment, type of ensemble, time boundaries etc); data will be retrieved and selected for each variable that is specified in the diagnostics section of the recipe;

# **DATA FIXING**

• the ESMValTool requires data to be in CMOR format; since errors in the data formatting are not uncommon, the ESMValTool performs checks against the CMOR library and fixes small irregularities (note that the degree of leniency is not very high).

### **SEVEN**

## VARIABLE DERIVATION

- variable derivation (in the case of non CMOR-standard variables, most likely associated with observational datasets) is performed automatically before running the preprocessor;
- if the variable definitions are already in the database then the user will just have to specify the variable to be derived in the diagnostics section (as any other standard variable, just setting derive: true).

# **RUN THE PREPROCESSOR**

- if any preprocessor section is specified in the recipe file, then data will be loaded in memory as iris cubes and passed through the preprocessing steps required by the user and specified in the preprocessor section, using the specific preprocessing step parameters provided by the user as keys (for the parameter name) and values (for the parameter value); the preprocessing order is very important since a number of steps depend on prior execution of other steps (e.g. multimodel statistics can not be computed unless all models are on a common grid, hence a prior regridding on a common grid is necessary); the preprocessor steps order can be set by the user as custom or the default order can be used;
- once preprocessing has finished, the tool writes the data output to disk as netCDF files so that the diagnostics can pick it up and use it; the user will also be provided with a metadata file containing a summary of the preprocessing and pointers to its output. Note that writing data to disk between the preprocessing and the diagnostic phase is required to ensure multi-language support for the latter.

## NINE

## **RUN THE DIAGNOSTICS**

• the last and most important phase can now be run: using output files from the preprocessor, the diagnostic scripts are executed using the provided diagnostics parameters.

# Part III

**Getting started** 

# INSTALLATION

**Note:** ESMValTool now uses *mamba* instead of *conda* for the recommended installation. For more information about the change, have a look at *Move to Mamba*.

ESMValTool supports Python 3.9 and later and requires Linux or MacOS. Successful usage on Windows has been reported by following the Linux installation instructions with WSL.

ESMValTool can be installed in multiple ways.

Recommended installation method:

Install the mamba package manager and then follow the instructions for

- ESMValTool installation on Linux
- ESMValTool installation on MacOS.

Further options for installation are:

- From the source code available at https://github.com/ESMValGroup/ESMValTool;
- From pre-installed versions on HPC clusters;
- Deployment through a Docker container (see https://www.docker.com);
- Deployment through a Singularity container (see https://sylabs.io/guides/latest/user-guide/);
- Installation with pip (see https://pypi.org);
- Installation from the conda lock file.

The next sections will detail the procedure to install ESMValTool through each of these methods.

There is also a lesson available in the ESMValTool tutorial that describes the installation of the ESMValTool in more detail. It can be found here.

See common installation issues if you run into trouble.

## 10.1 Mamba/Conda installation

In order to install ESMValTool and its dependencies from conda-forge, you will first need to install the mamba package manager. We recommend using mamba as a package manager for your conda environments instead of conda because it is much faster, see *move-to-mamba* for more information.

For a minimal mamba installation (recommended) go to https://mamba.readthedocs.io/en/latest/installation.html.

**Note:** It is recommended that you always use the latest version of mamba, as problems have been reported when trying to use older versions.

**Note:** Some systems provide a pre-installed version of conda or mamba (e.g. via the module environment). However, several users reported problems when installing with such versions. It is therefore preferable to use a local, fully user-controlled mamba installation.

First download the installation file for Linux or MacOSX. After downloading the installation file from one of the links above, execute it by running (Linux example):

bash Mambaforge-Linux-x86\_64.sh

and follow the instructions on your screen.

Note: Make sure to choose an installation location where you have at least 10 GB of disk space available.

During installation, mamba will ask you if you want mamba to be automatically loaded from your .bashrc or . bash-profile files. It is recommended that you answer yes. If you answered no, you can load the correct paths and environment variables later by running:

source <prefix>/etc/profile.d/conda.sh

where <prefix> is the installation location of mamba (e.g. /home/\$USER/mambaforge if you chose the default installation path).

If you use another shell than Bash, have a look at the available configurations in the <prefix>/etc/profile.d directory.

You can check that mamba installed correctly by running

which mamba

this should show the path to your mamba executable, e.g. ~/mambaforge/bin/mamba.

It is recommended to update both mamba and conda after installing:

mamba update --name base mamba conda

#### 10.1.1 ESMValTool installation on Linux

Once you have installed the mamba package manager, you can install the entire ESMValTool package by running:

mamba create --name esmvaltool esmvaltool

It is also possible to install just a subset of the ESMValTool dependencies by installing one or more of the *subpackages* described in the next section.

The command above will create a new conda environment called esmvaltool, and install ESMValTool in it. Of course it is also possible to choose a different name than esmvaltool for the environment.

**Note:** Creating a new conda environment is often much faster and more reliable than trying to update an existing conda environment. Therefore it is recommended that you create a new environment when you want to upgrade to the latest version.

The next step is to check that the installation works properly.

First activate the environment with the command:

conda activate esmvaltool

and then run the tool with the command:

esmvaltool --help

If everything was installed properly, ESMValTool should have printed a help message to the console.

#### 10.1.2 Installation of subpackages

The diagnostics bundled in ESMValTool are scripts in four different programming languages: Python, NCL, R, and Julia.

There are three language specific packages available:

- esmvaltool-ncl
- esmvaltool-python
- esmvaltool-r

The main esmvaltool package contains all three subpackages listed above. For the Julia dependencies, there is no subpackage yet, but there are special *installation instructions*. If you only need to run a recipe with diagnostics in some of these languages, it is possible to install only the dependencies needed to do just that. The diagnostic script(s) used in each recipe, are documented in *Recipes*. The extension of the diagnostic script can be used to see in which language a diagnostic script is written (.py for Python, .ncl for NCL, .R for R, and .jl for Julia diagnostics).

To install support for diagnostics written in Python and NCL into an existing environment, run

```
mamba install esmvaltool-python esmvaltool-ncl
```

Some of the CMORization scripts are written in Python, while others are written in NCL. Therefore, both esmvaltool-python and esmvaltool-ncl need to be installed in order to be able to run all CMORization scripts.

Note that the ESMValTool source code is contained in the esmvaltool-python package, so this package will always be installed as a dependency if you install one or more of the packages for other languages.

#### 10.1.3 Installation of Julia dependencies

If you want to use the ESMValTool Julia functionality, you will also need to install Julia. If you are just getting started, we suggest that you come back to this step later when, and if you need it. To perform the Julia installation, make sure that your conda environment is activated and then execute

```
mamba install julia
esmvaltool install Julia
```

#### 10.1.4 ESMValTool installation on MacOS

The Python diagnostics of the ESMValTool are supported on MacOS, but Julia, NCL, and R are not. If any of these are needed, deployment through a *Docker* container is advised.

The esmvaltool-python diagnostics can be installed as follows:

First, ensure mamba is installed (see install\_with\_mamba for more details).

Create a new environment with the esmvaltool-python package:

mamba create --name esmvaltool esmvaltool-python

Activate the new environment:

```
conda activate esmvaltool
```

Confirm that the ESMValTool is working with:

```
esmvaltool --help
```

Note that some recipes may depend on the OpenMP library, which does not install via mamba on MacOS. To install this library, run:

brew install libomp

to install the library with Homebrew. In case you do not have Homebrew, follow installation instructions here.

### 10.2 Install from source

Installing the tool from source is recommended if you need the very latest features or if you would like to contribute to its development.

Obtaining the source code

The ESMValTool source code is available on a public GitHub repository: https://github.com/ESMValGroup/ ESMValTool

The easiest way to obtain it is to clone the repository using git (see https://git-scm.com/). To clone the public repository:

```
git clone https://github.com/ESMValGroup/ESMValTool
```

or

git clone git@github.com:ESMValGroup/ESMValTool

if you prefer to connect to the repository over SSH.

The command above will create a folder called ESMValTool containing the source code of the tool in the current working directory.

**Note:** Using SSH is much more convenient if you push to the repository regularly (recommended to back up your work), because then you do not need to type your password over and over again. See this guide for information on how to set it up if you have not done so yet. If you are developing ESMValTool on a shared compute cluster, you can set up SSH agent forwarding to use your local SSH keys also from the remote machine.

It is also possible to work in one of the ESMValTool private repositories, e.g.:

```
git clone https://github.com/ESMValGroup/ESMValTool-private
```

GitHub also allows one to download the source code in as a tar.gz or zip file. If you choose to use this option, download the compressed file and extract its contents at the desired location.

#### Install dependencies

It is recommended to use mamba to manage ESMValTool dependencies. See the *mamba installation instructions* at the top of this page for instructions on installing mamba. To simplify the installation process, an environment definition file is provided in the repository (environment.yml in the root folder).

The ESMValTool conda environment file can also be used as a requirements list for those cases in which a mamba installation is not possible or advisable. From now on, we will assume that the installation is going to be done through mamba.

Ideally, you should create a separate conda environment for ESMValTool, so it is independent from any other Python tools present in the system.

To create an environment, go to the directory containing the ESMValTool source code that you just downloaded. It is called ESMValTool if you did not choose a different name.

```
cd ESMValTool
```

and create a new environment called esmvaltool with the command (when on Linux):

mamba env create --name esmvaltool --file environment.yml

```
or (when on MacOS)
```

mamba env create --name esmvaltool --file environment\_osx.yml

This will install all of the required development dependencies. Note that the MacOS environment file contains only Python dependencies, so you will not be able to run NCL, R, or Julia diagnostics with it.

**Note:** The environment is called esmvaltool in the example above, but it is possible to use the option --name some\_environment\_name to define a different name. This can be useful when you have an older ESMValTool installation that you would like to keep. It is recommended that you create a new environment when updating ESMValTool.

Next, activate the environment by using the command:

conda activate esmvaltool

**Attention:** From now on, we assume that the conda environment containing the development dependencies for ESMValTool is activated.

Install ESMValTool

Once all dependencies have been installed, ESMValTool itself can be installed by running the following command in the directory containing the ESMValTool source code (called ESMValTool if you did not choose a different name):

pip install --editable '.[develop]'

Using the --editable flag will cause the installer to create a symbolic link from the installation location to your source code, so any changes you make to the source code will immediately be available in the installed version of the tool.

If you would like to run Julia diagnostic scripts, you will need to install the ESMValTool Julia dependencies:

esmvaltool install Julia

The next step is to check that the installation works properly. To do this, run the tool with:

esmvaltool --help

If everything was installed properly, ESMValTool should have printed a help message to the console.

**Note:** MacOS users: some recipes may depend on the OpenMP library, which does not install via mamba on MacOS. Instead run

brew install libomp

to install the library with Homebrew. In case you do not have Homebrew, follow installation instructions here.

For a more complete installation verification, run the automated tests and confirm that no errors are reported:

pytest -m "not installation"

or if you want to run the full test suite remove the -m "not installation" flag; also if you want to run the tests on multiple threads, making the run faster, use the -n N flag where N is the number of available threads e.g.

pytest -n 4

This concludes the installation from source guide. However, if you would like to do development work on ESMValCore, please read on.

## 10.2.1 Using the development version of the ESMValCore package

If you need the latest developments of the ESMValCore package, you can install it from source into the same conda environment.

Attention: The recipes and diagnostics in the ESMValTool repository are compatible with the latest released version of the ESMValCore. Using the development version of the ESMValCore package is only recommended if you are planning to develop new features for the ESMValCore, e.g. you want to implement a new preprocessor function.

First follow the steps in the section above to *install ESMValTool from source*. Next, go to the place where you would like to keep the source code and clone the ESMValCore github repository:

git clone https://github.com/ESMValGroup/ESMValCore

or

git clone git@github.com:ESMValGroup/ESMValCore

The command above will create a folder called ESMValCore containing the source code of the tool in the current working directory.

Go into the folder you just downloaded

cd ESMValCore

and then install ESMValCore in development mode

```
pip install --editable '.[develop]'
```

To check that the installation was successful, run

python -c 'import esmvalcore; print(esmvalcore.\_\_path\_\_[0])'

this should show the directory of the source code that you just downloaded.

If the command above shows a directory inside your conda environment instead, e.g. ~/mambaforge/envs/ esmvaltool/lib/python3.9/site-packages/esmvalcore, you may need to manually remove that directory and run pip install --editable '.[develop]' again.

## 10.3 Pre-installed versions on HPC clusters / other servers

ESMValTool is available on the HPC clusters CEDA-JASMIN and DKRZ-Levante, and on the Met Office Linux estate, so there is no need to install ESMValTool if you are just running recipes:

- CEDA-JASMIN: *esmvaltool* is available on the scientific compute nodes (*sciX.jasmin.ac.uk* where X = 1, 2, 3, 4, 5) after login and module loading via *module load esmvaltool*; see the helper page at CEDA.
- DKRZ-Levante: *esmvaltool* is available on login nodes (*levante.dkrz.de*) after login and module loading via *module load esmvaltool*; the command *module help esmvaltool* provides some information about the module. A Jupyter kernel based on the latest module is available from DKRZ-JupyterHub.
- Met Office: *esmvaltool* is available on the Linux estate after login and module loading via *module load*; see the ESMValTool Community of Practice SharePoint site for more details.

The ESMValTool Tutorial provides a quickstart guide that is particularly suited for new users that have an access to pre-installed version of ESMValTool.

Information on how to request an account at CEDA-JASMIN and DKRZ-Levante and to get started with these HPC clusters can be found on the setup page of the tutorial here.

# **10.4 Docker installation**

ESMValTool is also provided through DockerHub in the form of docker containers. See https://docs.docker.com for more information about docker containers and how to run them.

You can get the latest release with

docker pull esmvalgroup/esmvaltool:stable

If you want to use the current main branch, use

```
docker pull esmvalgroup/esmvaltool:latest
```

To run a container using those images, use:

docker run esmvalgroup/esmvaltool:stable --help

Note that the container does not see the data or environmental variables available in the host by default. You can make data available with -v /path:/path/in/container and environmental variables with -e VARNAME.

For example, the following command would run a recipe

```
docker run -e HOME -v "$HOME":"$HOME" -v /data:/data esmvalgroup/esmvaltool:stable run_
→examples/recipe_python.yml
```

with the environmental variable \$HOME available inside the container and the data in the directories \$HOME and /data, so these can be used to find the configuration file, recipe, and data.

It might be useful to define a bash alias or script to abbreviate the above command, for example

```
alias esmvaltool="docker run -e HOME -v $HOME:$HOME -v /data:/data esmvalgroup/

→esmvaltool:stable"
```

would allow using the esmvaltool command without even noticing that the tool is running inside a Docker container.

# 10.5 Singularity installation

Docker is usually forbidden in clusters due to security reasons. However, there is a more secure alternative to run containers that is usually available on them: Singularity.

Singularity can use docker containers directly from DockerHub with the following command

singularity run docker://esmvalgroup/esmvaltool:stable run examples/recipe\_python.yml

Note that the container does not see the data available in the host by default. You can make host data available with -B /path:/path/in/container.

It might be useful to define a bash alias or script to abbreviate the above command, for example

```
alias esmvaltool="singularity run -B $HOME:$HOME -B /data:/data docker://esmvalgroup/

→esmvaltool:stable"
```

would allow using the esmvaltool command without even noticing that the tool is running inside a Singularity container. Some clusters may not allow to connect to external services, in those cases you can first create a singularity image locally:

singularity build esmvaltool.sif docker://esmvalgroup/esmvaltool:stable

and then upload the image file esmvaltool.sif to the cluster. To run the container using the image file esmvaltool. sif use:

singularity run esmvaltool.sif run examples/recipe\_python.yml

# 10.6 Pip installation

It is also possible to install ESMValTool from PyPI. However, this requires first installing dependencies that are not available on PyPI in some other way. The list of required dependencies can be found in environment.yml.

**Warning:** It is recommended to use the installation with mamba instead, as it may not be easy to install the correct versions of all dependencies.

After installing the dependencies that are not available from PyPI, install ESMValTool and any remaining Python dependencies with the command:

pip install esmvaltool

If you would like to run Julia diagnostic scripts, you will also need to install the Julia dependencies:

esmvaltool install Julia

## 10.7 Installation from the conda lock file

The conda lock file is an alternative to the environment.yml file used in the *installation from source instructions*. All other steps in those installation instructions are the same.

The conda lock file can be used to install the dependencies of ESMValTool whenever the conda environment defined by environment.yml can not be solved for some reason. A conda lock file is a reproducible environment file that contains links to dependency packages as they are hosted on the Anaconda cloud; these have frozen version numbers, build hashes, and channel names. These parameters are established at the time of the conda lock file creation, so may be outdated after a while. Therefore, we regenerate these lock files every 10 days through automatic Pull Requests (or more frequently, since the automatic generator runs on merges on the main branch too), to minimize the risk of dependencies becoming outdated.

Conda environment creation from a lock file is done with the following command:

conda create --name esmvaltool --file conda-linux-64.lock

The latest, most up-to-date file can always be downloaded directly from the source code repository, a direct download link can be found here.

Note: For instructions on how to manually create the lock file, see these instructions.

# 10.8 Common installation problems and their solutions

## 10.8.1 Mamba fails to solve the environment

If you see the text Solving environment: with the characters  $-\langle | / | rotating behind it for more than 10 minutes, mamba may be having problems finding a working combination of versions of the packages that the ESMValTool depends on. Because the ESMValTool is a community tool, there is no strict selection of which tools can be used and installing the ESMValTool requires installing almost any package that is available for processing climate data. To help mamba solve the environment, you can try the following.$ 

Always use the latest version of mamba, as problems have been reported by people using older versions, to update, run:

```
mamba update --name base mamba
```

Usually mamba is much better at solving new environments than updating older environments, so it is often a good idea to create a new environment if updating does not work.

It can help mamba if you let it know what version of certain packages you want, for example by running

mamba create -n esmvaltool esmvaltool 'python=3.11'

you ask for Python 3.11 specifically and that makes it much easier for mamba to solve the environment, because now it can ignore any packages that were built for other Python versions. Note that, since the esmvaltool package is built with Python>=3.9, asking for an older Python version, e.g. *python=3.7*, in this way, it will result in installation failure.

## **10.8.2 Problems with proxies**

If you are installing ESMValTool from source from behind a proxy that does not trust the usual PyPI URLs you can declare them with the option --trusted-host, e.g.

```
pip install --trusted-host=pypi.python.org --trusted-host=pypi.org --trusted-host=files.
→pythonhosted.org -e .[develop]
```

If R packages fail to download, you might be able to solve this by setting the environment variable http\_proxy to the correct value, e.g. in bash:

export http\_proxy=http://user:pass@proxy\_server:port

the username and password can be omitted if they are not required. See e.g. here for more information.

## **10.8.3 Anaconda servers connection issues**

HTTP connection errors (of e.g. type 404) to the Anaconda servers are rather common, and usually a retry will solve the problem.

## 10.8.4 Installation of R packages fails

Problems have been reported if the R interpreter was made available through the module load command in addition to installation from mamba. If your ESMValTool conda environment is called esmvaltool and you want to use the R interpreter installed from mamba, the path to the R interpreter should end with mamba/envs/esmvaltool/bin/R or conda/envs/esmvaltool/bin/R. When the conda environment for ESMValTool is activated, you can check which R interpreter is used by running

which R

The Modules package is often used by system administrators to make software available to users of scientific compute clusters. To list any currently loaded modules run module list, run module help or man module for more information about the Modules package.

## 10.8.5 Problems when using ssh

If you log in to a cluster or other device via SSH and your origin machine sends the locale environment via the SSH connection, make sure the environment is set correctly, specifically LANG and LC\_ALL are set correctly (for GB English UTF-8 encoding these variables must be set to en\_GB.UTF-8; you can set them by adding export LANG=en\_GB.UTF-8 and export LC\_ALL=en\_GB.UTF-8) in your origin or login machines' .profile.

## 10.8.6 Problems when updating the conda environment

Usually mamba is much better at solving new environments than updating older environments, so it is often a good idea to create a new environment if updating does not work. See also *Mamba fails to solve the environment*.

Do not run mamba update --update-all in the esmvaltool environment since that will update some packages that are pinned to specific versions for the correct functionality of the tool.

# 10.9 Move to Mamba

Mamba is a much faster alternative to *conda*, and environment creation and updating benefits from the use of a much faster (C++ backend) dependency solver; tests have been performed to verify the integrity of the *esmvaltool* environment built with *mamba*, and we are now confident that the change will not affect the way ESMValTool is installed and run, whether it be on a Linux or OS platform. From the user's perspective, it is a straightforward use change: the CLI (command line interface) of *mamba* is identical to *conda*: any command that was run with *conda* before will now be run with *mamba* instead, keeping all the other command line arguments and flags as they were before. The only place where *conda* should not be replaced with *mamba* at command line level is at the environment activation point: *conda activate* will still have to be used.

## CHAPTER

## **ELEVEN**

# CONFIGURATION

The esmvaltool command is provided by the ESMValCore package, the documentation on configuring ESMValCore can be found here. In particular, it is recommended to read the section on the User configuration file and the section on Finding data.

To install the default configuration file in the default location, run

esmvaltool config get\_config\_user

Note that this file needs to be customized using the instructions above, so the esmvaltool command can find the data on your system, before it can run a recipe.

There is a lesson available in the ESMValTool tutorial that describes how to personalize the configuration file. It can be found at this site.

## CHAPTER

## TWELVE

# RUNNING

ESMValTool is mostly used as a command line tool. Whenever your Conda environment for ESMValTool is active, you can run the command esmvaltool. See running esmvaltool in the ESMValCore documentation for an introduction to the esmvaltool command.

# 12.1 Running your first recipe

There is a step-by-step tutorial available in the ESMValTool tutorial on how to run your first recipe. It can be found here.

An example recipe is available in the ESMValTool installation folder as examples/recipe\_python.yml.

This recipe finds data from BCC-ESM1 and CanESM2 and creates two plot types:

- a global map plot that shows the monthly mean 2m surface air temperature in January 2000.
- a time series plot that shows the globally averaged annual mean 2m surface air temperature and compares it to the one in Amsterdam.

To run this recipe and automatically download the required climate data from ESGF to the local directory ~/ climate\_data, run

esmvaltool run examples/recipe\_python.yml --search\_esgf=when\_missing

The --search\_esgf=when\_missing option tells ESMValTool to search for and download the necessary climate data files, if they cannot be found locally. The data only needs to be downloaded once, every following run will re-use previously downloaded data. If you have all required data available locally, you can run the tool with --search\_esgf=never argument (the default). Note that in that case the required data should be located in the directories specified in your user configuration file. A third option --search\_esgf=always is available. With this option, the tool will first check the ESGF for the needed data, regardless of any local data availability; if the data found on ESGF is newer than the local data (if any) or the user specifies a version of the data that is available only from the ESGF, then that data will be downloaded; otherwise, local data will be used. Recall that the chapter *Configuring ESMValTool* provides an explanation of how to create your own config-user.yml file.

See running esmvaltool in the ESMValCore documentation for a more complete introduction to the esmvaltool command.

# 12.2 Available diagnostics and metrics

Although ESMValTool can be used to download data, analyze it using ESMValCore's preprocessing modules, and the creation of your own analysis code, its main purpose is the continuously growing set of diagnostics and metrics that it directly provides to the user. These metrics and diagnostics are provided as a set of preconfigured recipes that users can run or customize for their own analysis. The latest list of available recipes can be found here.

In order to make the management of these installed recipes easier, ESMValTool provides the recipes command group with utilities that help the users in discovering and customizing the provided recipes.

The first command in this group allows users to get the complete list of installed recipes printed to the console:

esmvaltool recipes list

If the user then wants to explore any one of these recipes, they can be printed using the following command

esmvaltool recipes show recipe\_name.yml

Note that there is no recipe\_name.yml shipped with ESMValTool, replace this with a recipes that is available, for example examples/recipe\_python.yml. Finally, to get a local copy that can then be customized and run, users can run the following command

esmvaltool recipes get recipe\_name.yml

Note that the esmvaltool run recipe\_name.yml command will first look if recipe\_name.yml is the path to an existing file. If this is the case, it will run that recipe. If not, it will look if it is a relative path to an existing recipe with respect to the recipes directory in your ESMValTool installation and run that.

# 12.3 Running multiple recipes

Have a look at Running multiple recipes if you are interested in running multiple recipes in parallel.

## CHAPTER

## THIRTEEN

# OUTPUT

ESMValTool automatically generates a new output directory with every run. The location is determined by the output\_dir option in the config-user.yml file, the recipe name, and the date and time, using the the format: YYYYM-MDD\_HHMMSS.

For instance, a typical output location would be: output\_directory/recipe\_ocean\_amoc\_20190118\_1027/

This is effectively produced by the combination: output\_dir/recipe\_name\_YYYYMMDD\_HHMMSS/

This directory will contain 4 further subdirectories:

- 1. *Diagnostic output* (work): A place for any diagnostic script results that are not plots, e.g. files in NetCDF format (depends on the diagnostics).
- 2. *Plots*: The location for all the plots, split by individual diagnostics and fields.
- 3. *Run*: This directory includes all log files, a copy of the recipe, a summary of the resource usage, and the *set*-*tings.yml* interface files and temporary files created by the diagnostic scripts.
- 4. *Preprocessed datasets* (preproc): This directory contains all the preprocessed netcdfs data and the *metadata.yml* interface files. Note that by default this directory will be deleted after each run, because most users will only need the results from the diagnostic scripts.

# **13.1 Preprocessed datasets**

The preprocessed datasets will be stored to the preproc/ directory. Each variable in each diagnostic will have its own the *metadata.yml* interface files saved in the preproc directory.

If the option save\_intermediary\_cubes is set to true in the config-user.yml file, then the intermediary cubes will also be saved here. This option is set to false in the default config-user.yml file.

If the option remove\_preproc\_dir is set to true in the config-user.yml file, then the preproc directory will be deleted after the run completes. This option is set to true in the default config-user.yml file.

## 13.2 Run

The log files in the run directory are automatically generated by ESMValTool and create a record of the output messages produced by ESMValTool and they are saved in the run directory. They can be helpful for debugging or monitoring the job, but also allow a record of the job output to screen after the job has been completed.

The run directory will also contain a copy of the recipe and the *settings.yml* file, described below. The run directory is also where the diagnostics are executed, and may also contain several temporary files while diagnostics are running.

# 13.3 Diagnostic output

The work/ directory will contain all files that are output at the diagnostic stage. Ie, the model data is preprocessed by ESMValTool and stored in the preproc/ directory. These files are opened by the diagnostic script, then some processing is applied. Once the diagnostic level processing has been applied, the results should be saved to the work directory.

# 13.4 Plots

The plots directory is where diagnostics save their output figures. These plots are saved in the format requested by the option *output\_file\_type* in the config-user.yml file.

# 13.5 Settings.yml

The settings.yml file is automatically generated by ESMValCore. For each diagnostic, a unique settings.yml file will be produced.

The settings.yml file passes several global level keys to diagnostic scripts. This includes several flags from the configuser.yml file (such as 'write\_netcdf', 'write\_plots', etc...), several paths which are specific to the diagnostic being run (such as 'plot\_dir' and 'run\_dir') and the location on disk of the metadata.yml file (described below).

```
input_files:[[...]recipe_ocean_bgc_20190118_134855/preproc/diag_timeseries_scalars/mfo/
→metadata.yml]
log_level: debug
output_file_type: png
plot_dir: [...]recipe_ocean_bgc_20190118_134855/plots/diag_timeseries_scalars/Scalar_
→timeseries
profile_diagnostic: false
recipe: recipe_ocean_bgc.yml
run_dir: [...]recipe_ocean_bgc_20190118_134855/run/diag_timeseries_scalars/Scalar_
→timeseries
script: Scalar_timeseries
version: 2.0a1
work_dir: [...]recipe_ocean_bgc_20190118_134855/work/diag_timeseries_scalars/Scalar_
→timeseries
write_netcdf: true
write_plots: true
```

The first item in the settings file will be a list of *Metadata.yml* files. There is a metadata.yml file generated for each field in each diagnostic.

# 13.6 Metadata.yml

The metadata.yml files is automatically generated by ESMValTool. Along with the settings.yml file, it passes all the paths, boolean flags, and additional arguments that your diagnostic needs to know in order to run.

The metadata is loaded from cfg as a dictionary object in python diagnostics.

Here is an example metadata.yml file:

```
?
  [...]/recipe_ocean_bgc_20190118_134855/preproc/diag_timeseries_scalars/mfo/CMIP5_
→HadGEM2-ES_Omon_historical_r1i1p1_T00M_mfo_2002-2004.nc
  : cmor_table: CMIP5
 dataset: HadGEM2-ES
 diagnostic: diag_timeseries_scalars
 end_year: 2004
 ensemble: r1i1p1
 exp: historical
 field: TOOM
 filename: [...]recipe_ocean_bgc_20190118_134855/preproc/diag_timeseries_scalars/mfo/
→CMIP5_HadGEM2-ES_Omon_historical_r1i1p1_T00M_mfo_2002-2004.nc
 frequency: mon
 institute: [INPE, MOHC]
 long_name: Sea Water Transport
 mip: Omon
 modeling_realm: [ocean]
 preprocessor: prep_timeseries_scalar
 project: CMIP5
 recipe_dataset_index: 0
 short_name: mfo
 standard_name: sea_water_transport_across_line
 start_year: 2002
 units: kg s-1
 variable_group: mfo
```

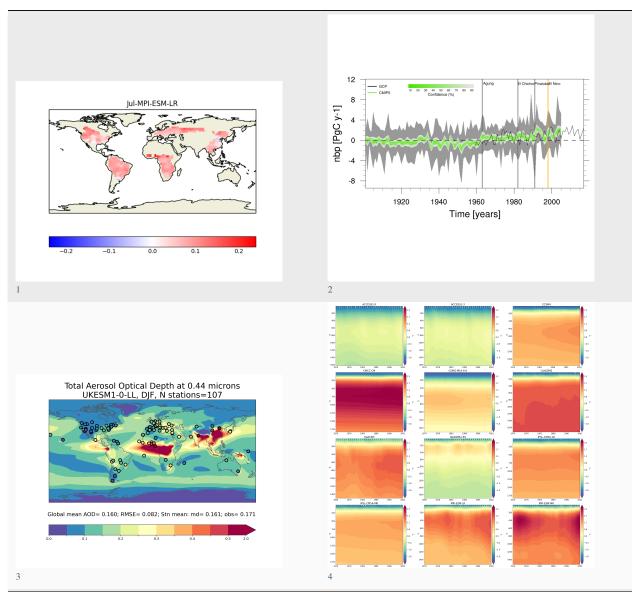
As you can see, this is effectively a dictionary with several items including data paths, metadata and other information.

There are several tools available in python which are built to read and parse these files. The tools are available in the shared directory in the diagnostics directory.

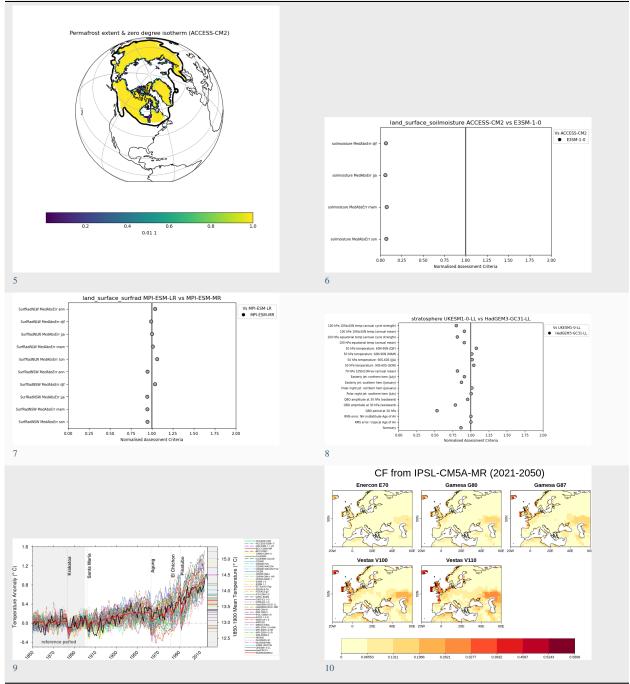
# Part IV

# Gallery

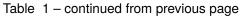
This section shows example plots produced by ESMValTool. For more information, click on the footnote below the image. A website displaying results produced with the latest release of ESMValTool for all available recipes can be accessed here.

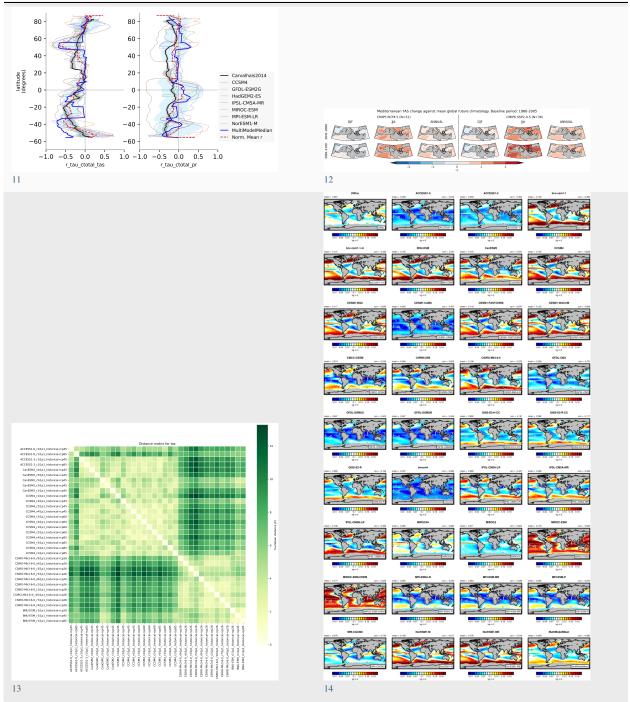


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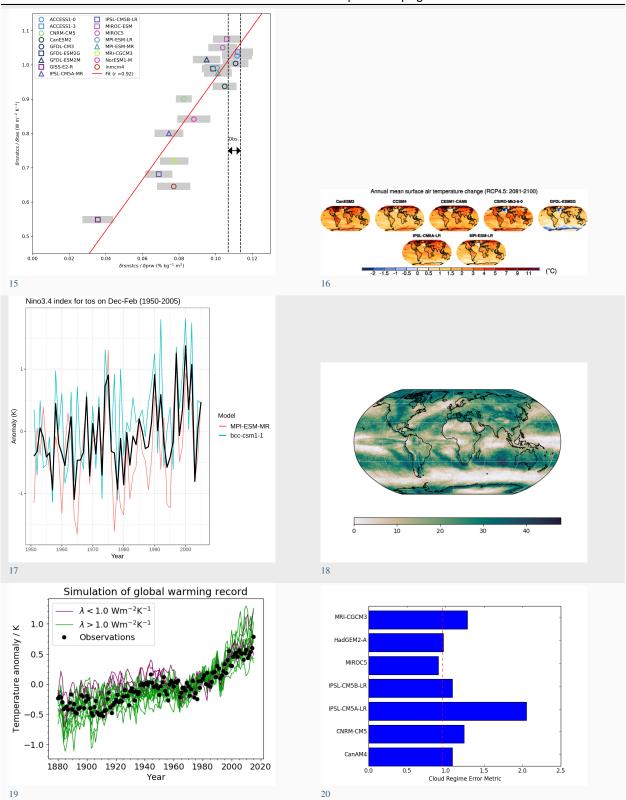


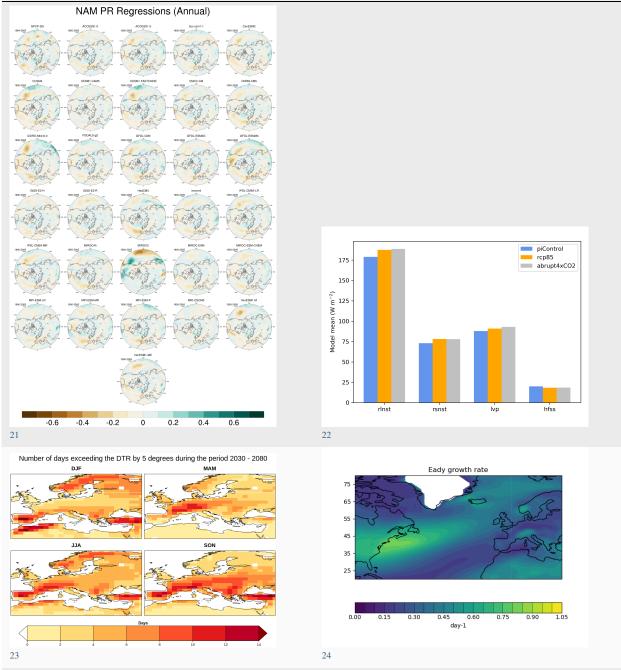
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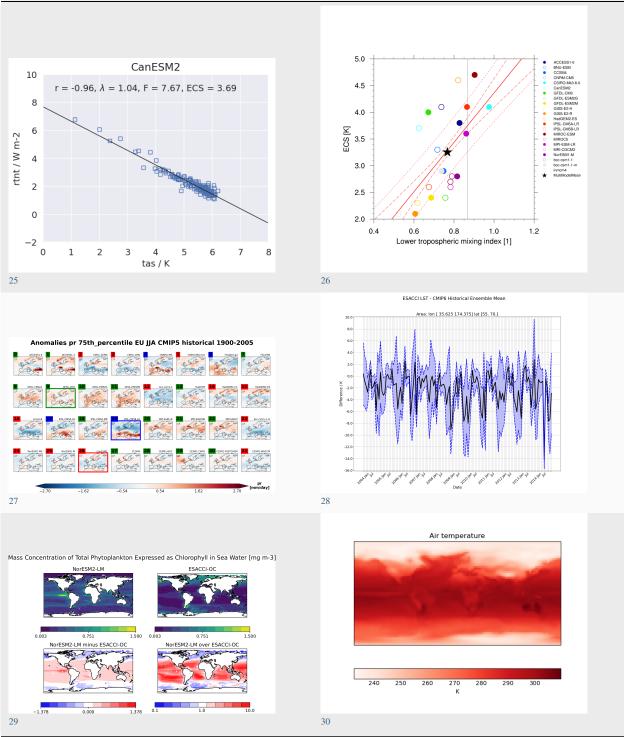
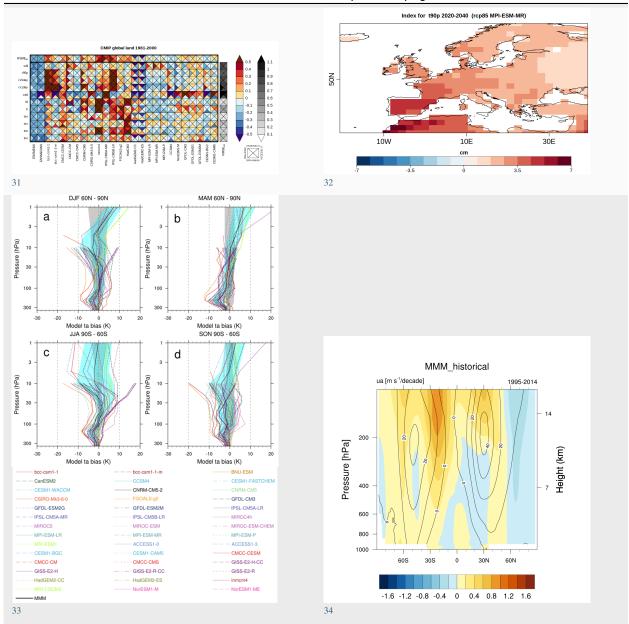
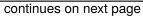
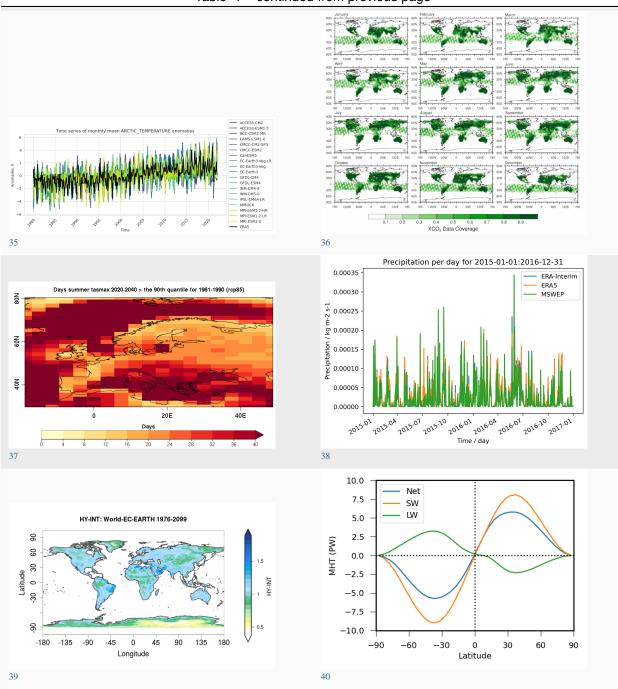
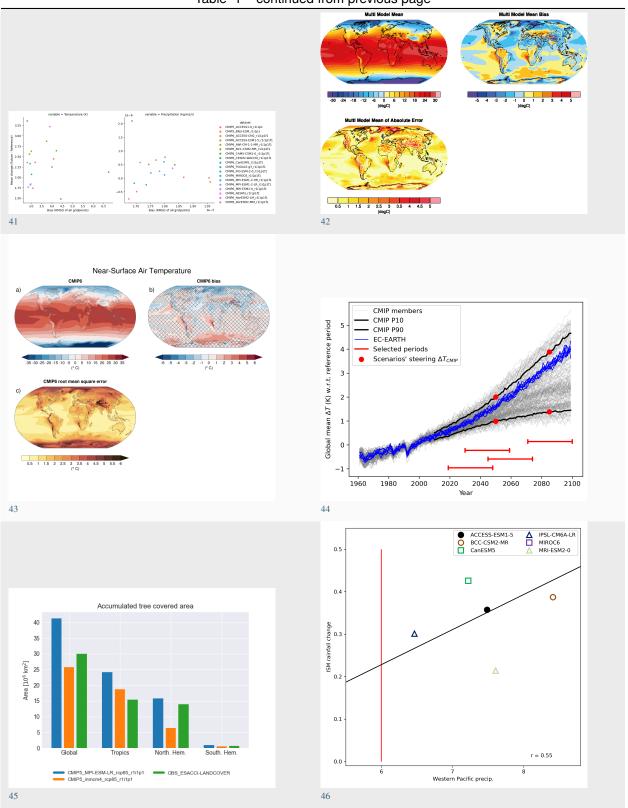


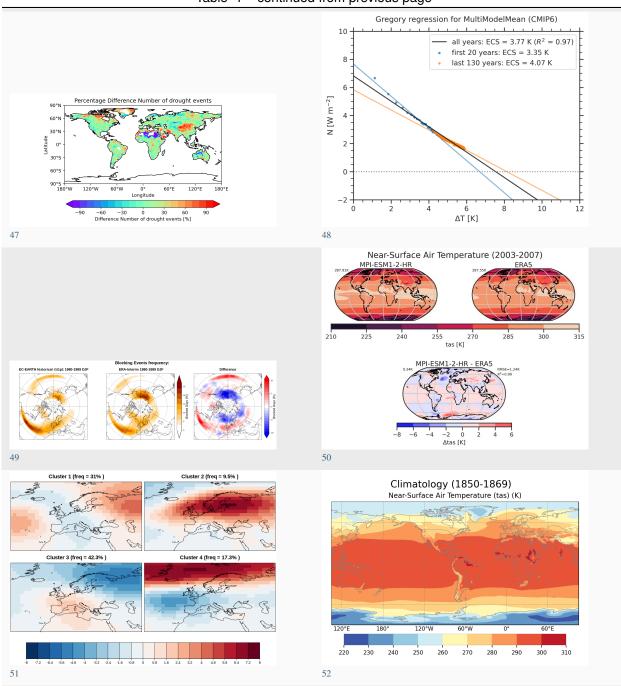
Table 1 – continued from previous page











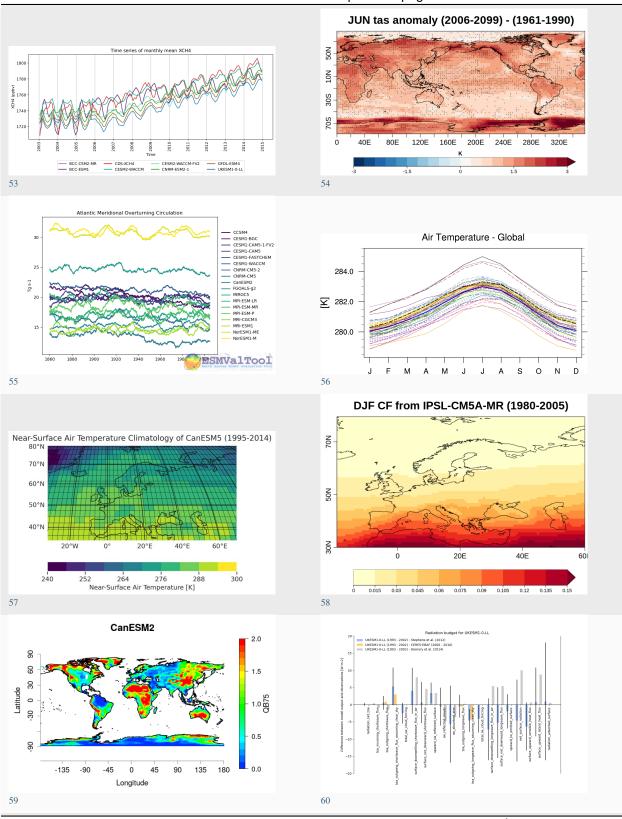


Table 1 - continued from previous page

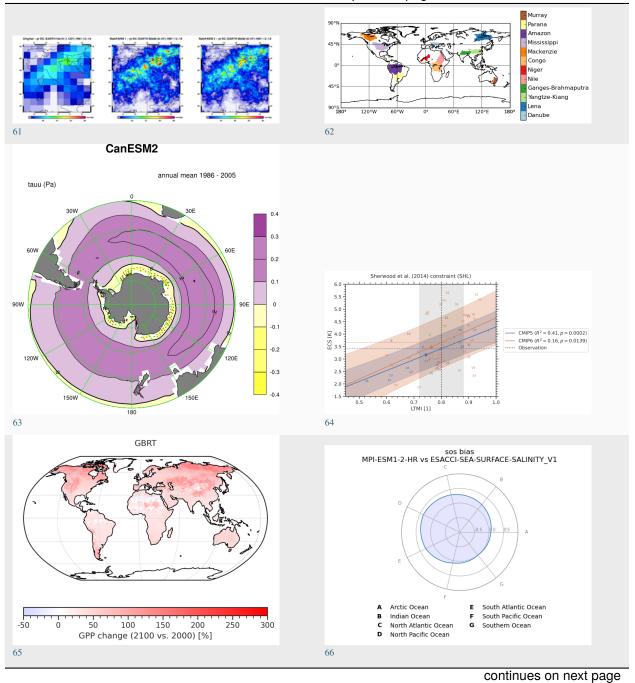
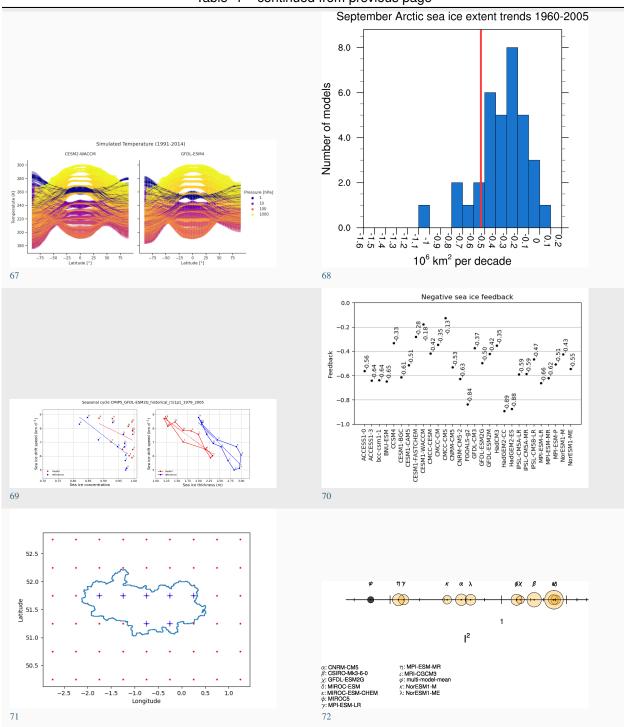


Table 1 – continued from previous page



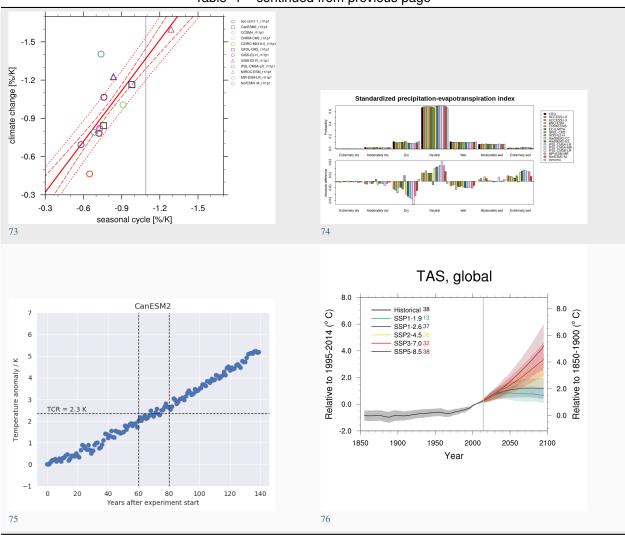
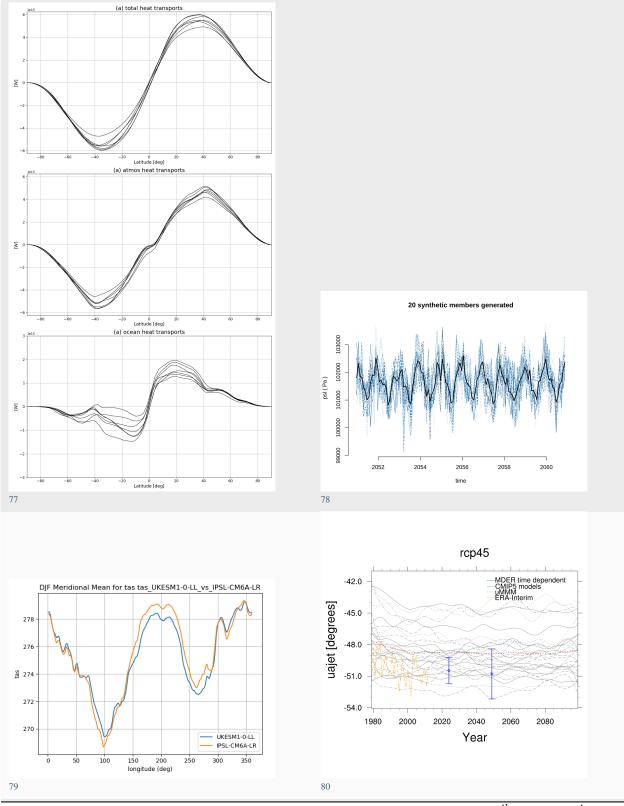
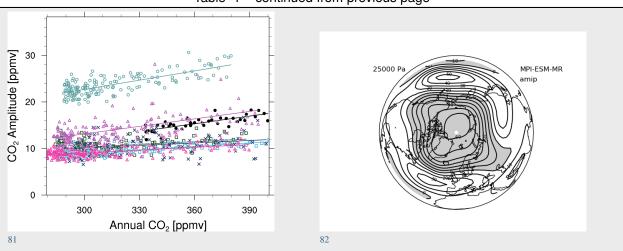


Table 1 – continued from previous page

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- <sup>1</sup> Landcover Albedo
- <sup>2</sup> Land and ocean components of the global carbon cycle
- <sup>3</sup> AOD AeroNET Assess
- <sup>4</sup> Recipe for evaluating Arctic Ocean
- <sup>5</sup> Land-surface Permafrost Autoassess diagnostics
- <sup>6</sup> Land-surface Soil Moisture Autoassess diagnostics
- <sup>7</sup> Land-surface Surface Radiation Autoassess diagnostics
- <sup>8</sup> Stratosphere Autoassess diagnostics
- <sup>9</sup> Quantifying progress across different CMIP phases
- <sup>10</sup> Capacity factor of wind power: Ratio of average estimated power to theoretical maximum power
- <sup>11</sup> Turnover time of carbon over land ecosystems
- <sup>12</sup> Climate Change Hotspot
- <sup>13</sup> Climate model Weighting by Independence and Performance (ClimWIP)
- <sup>14</sup> Clouds
- <sup>15</sup> Evaluate water vapor short wave radiance absorption schemes of ESMs with the observations, including ESACCI data.
- <sup>16</sup> IPCC AR5 Chapter 12 (selected figures)
- <sup>17</sup> Nino indices, North Atlantic Oscillation (NAO), Souther Oscillation Index (SOI)
- <sup>18</sup> Consecutive dry days
- <sup>19</sup> Emergent constraint on equilibrium climate sensitivity from global temperature variability
- <sup>20</sup> Cloud Regime Error Metric (CREM)
- <sup>21</sup> Climate Variability Diagnostics Package (CVDP)
- <sup>22</sup> Evaluate water vapor short wave radiance absorption schemes of ESMs with the observations.
- <sup>23</sup> Diurnal temperature range
- <sup>24</sup> Eady growth rate
- <sup>25</sup> Equilibrium climate sensitivity
- <sup>26</sup> Emergent constraints for equilibrium climate sensitivity
- <sup>27</sup> Ensemble Clustering a cluster analysis tool for climate model simulations (EnsClus)
- <sup>28</sup> ESA CCI LST comparison to Historical Models
- <sup>29</sup> Ocean chlorophyll in ESMs compared to ESA-CCI observations.
- <sup>30</sup> Example recipes
- <sup>31</sup> Extreme Events Indices (ETCCDI)
- <sup>32</sup> Combined Climate Extreme Index
- <sup>33</sup> Diagnostics of stratospheric dynamics and chemistry
- <sup>34</sup> Ozone and associated climate impacts
- <sup>35</sup> Timeseries for Arctic-Midlatitude Teleconnections
- <sup>36</sup> Spatially resolved evaluation of ESMs with satellite column-averaged CO2
- 37 Heat wave and cold wave duration
- <sup>38</sup> Hydro forcing comparison
- <sup>39</sup> Hydroclimatic intensity and extremes (HyInt)
- <sup>40</sup> Implied heat transport from Top of Atmosphere fluxes
- <sup>41</sup> Quick insights for climate impact researchers
- <sup>42</sup> *IPCC AR5 Chapter 9 (selected figures)*
- <sup>43</sup> IPCC AR6 Chapter 3 (selected figures)
- <sup>44</sup> KNMI Climate Scenarios 2014
- <sup>45</sup> Landcover diagnostics
- <sup>46</sup> Constraining future Indian Summer Monsoon projections with the present-day precipitation over the tropical western Pacific
- <sup>47</sup> Drought characteristics following Martin (2018)
- <sup>48</sup> Context for interpreting equilibrium climate sensitivity and transient climate response from the CMIP6 Earth system models
- <sup>49</sup> Blocking metrics and indices, teleconnections and weather regimes (MiLES)
- <sup>50</sup> General model evaluation
- <sup>51</sup> Modes of variability
- <sup>52</sup> Monitor
- <sup>53</sup> Diagnostics of integrated atmospheric methane (XCH4)
- 54 Multi-model products
- 55 Ocean diagnostics
- <sup>56</sup> Performance metrics for essential climate parameters
- 57 Psyplot Diagnostics
- 58 Capacity factor for solar photovoltaic (PV) systems
- <sup>59</sup> Precipitation quantile bias
- 60 Radiation Budget
- <sup>61</sup> RainFARM stochastic downscaling
- <sup>62</sup> Runoff, Precipitation, Evapotranspiration
- <sup>63</sup> Ocean metrics
- <sup>64</sup> Emergent constraints on equilibrium climate sensitivity in CMIP5: do they hold for CMIP6?
- <sup>65</sup> Constraining uncertainty in projected gross primary production (GPP) with machine learning
- <sup>66</sup> Sea Surface Salinity Evaluation
- 67 Seaborn Diagnostics
- 68 Sea Ice
- <sup>69</sup> Seaice drift
- <sup>70</sup> Seaice feedback
- 71 Shapeselect
- <sup>72</sup> Single Model Performance Index (SMPI)
- <sup>73</sup> Emergent constraint on snow-albedo effect
- 74 Standardized Precipitation Evapotranspiration Index (SPEI)

Part V

# Recipes

A website displaying results produced with the latest release of ESMValTool for all available recipes can be accessed here.

CHAPTER

# FOURTEEN

# **GENERAL-PURPOSE DIAGNOSTICS**

Recipes that use highly customizable diagnostics which are designed to plot a large variety of input data.

# 14.1 General model evaluation

# 14.1.1 Overview

These recipes and diagnostics provide a basic climate model evaluation with observational data. This is especially useful to get an overview of the performance of a simulation. The diagnostics used here allow plotting arbitrary preprocessor output, i.e., arbitrary variables from arbitrary datasets.

# 14.1.2 Available recipes and diagnostics

Recipes are stored in recipes/model\_evaluation

- recipe\_model\_evaluation\_basics.yml
- recipe\_model\_evaluation\_clouds\_clim.yml
- recipe\_model\_evaluation\_clouds\_cycles.yml
- recipe\_model\_evaluation\_precip\_zonal.yml

Diagnostics are stored in *diag\_scripts/monitor/* 

• *multi\_datasets.py*: Monitoring diagnostic to show multiple datasets in one plot (incl. biases).

# 14.1.3 User settings

It is recommended to use a vector graphic file type (e.g., SVG) for the output format when running this recipe, i.e., run the recipe with the command line option --output\_file\_type=svg or use output\_file\_type: svg in your User configuration file. Note that map and profile plots are rasterized by default. Use rasterize: false in the recipe to disable this.

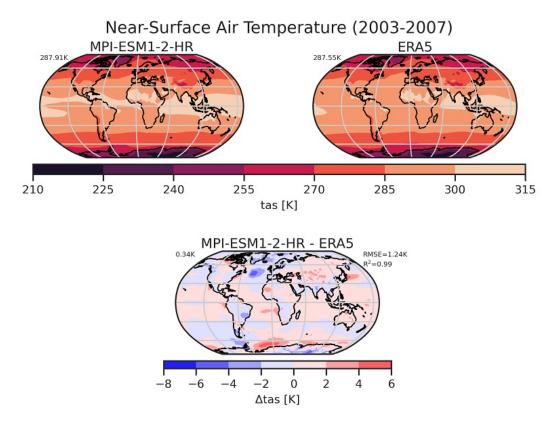
#### **Recipe settings**

A list of all possible configuration options that can be specified in the recipe is given for each diagnostic individually (see links given for the available diagnostics in the previous section).

# 14.1.4 Variables

Any, but the variables' number of dimensions should match the ones expected by each diagnostic (see links given for the available diagnostics in the previous section).

# 14.1.5 Example plots



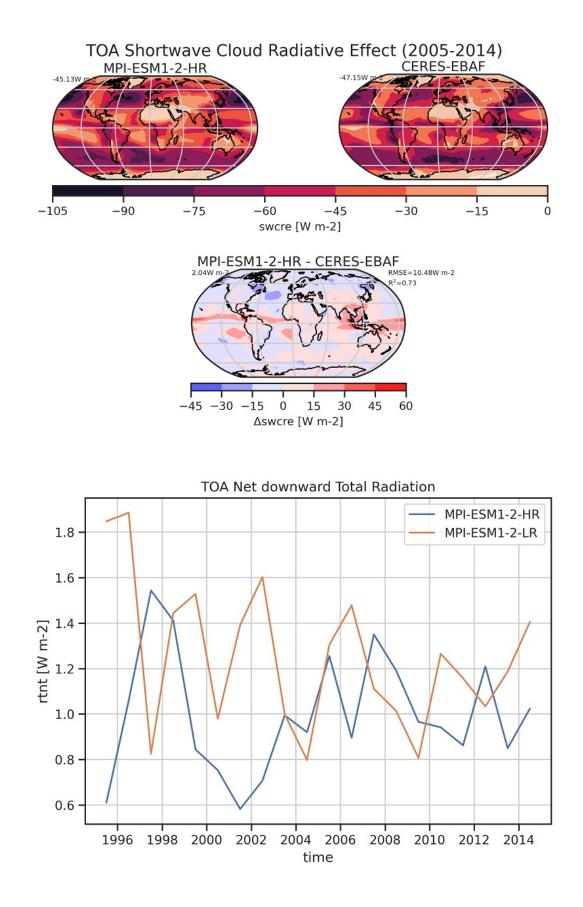
Global climatology of 2m near-surface air temperature.

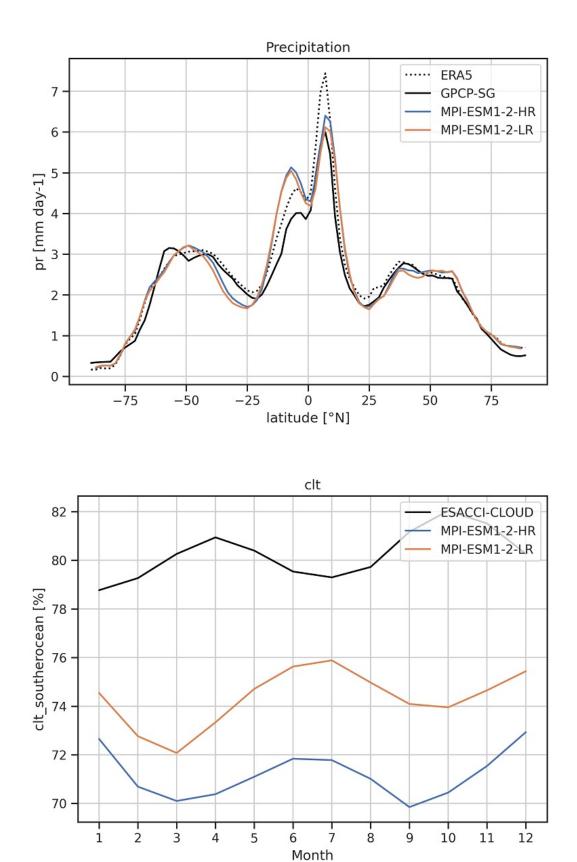
Global climatology of the shortwave cloud radiative effect (SWCRE).

Time series of the global mean top-of-the-atmosphere net radiative flux.

Zonal mean precipitation.

Annual cycle of Southern Ocean total cloud cover.





# 14.2 Monitor

# 14.2.1 Overview

These recipes and diagnostics allow plotting arbitrary preprocessor output, i.e., arbitrary variables from arbitrary datasets. In addition, a *base class* is provided that allows a convenient interface for all monitoring diagnostics.

# 14.2.2 Available recipes and diagnostics

Recipes are stored in *recipes/monitor* 

- recipe\_monitor.yml
- recipe\_monitor\_with\_refs.yml

Diagnostics are stored in *diag\_scripts/monitor/* 

- *monitor.py*: Monitoring diagnostic to plot arbitrary preprocessor output.
- compute\_eofs.py: Monitoring diagnostic to plot EOF maps and associated PC timeseries.
- *multi\_datasets.py*: Monitoring diagnostic to show multiple datasets in one plot (incl. biases).

# 14.2.3 User settings

It is recommended to use a vector graphic file type (e.g., SVG) for the output files when running this recipe, i.e., run the recipe with the command line option --output\_file\_type=svg or use output\_file\_type: svg in your User configuration file. Note that map and profile plots are rasterized by default. Use rasterize\_maps: false or rasterize: false (see *Recipe settings*) in the recipe to disable this.

#### **Recipe settings**

A list of all possible configuration options that can be specified in the recipe is given for each diagnostic individually (see previous section).

#### Monitor configuration file

In addition, the following diagnostics support the use of a dedicated monitor configuration file:

- monitor.py
- compute\_eofs.py

This file is a yaml file that contains map and variable specific options in two dictionaries maps and variables.

Each entry in maps corresponds to a map definition. Example:

```
maps:
  global: # Map name, choose a meaningful one
    projection: PlateCarree # Cartopy projection to use
    projection_kwargs: # Dictionary with Cartopy's projection keyword arguments.
        central_longitude: 285
        smooth: true # If true, interpolate values to get smoother maps. If not, all_
        →points in a cells will get the exact same color
```

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```
lon: [-120, -60, 0, 60, 120, 180] # Set longitude ticks
lat: [-90, -60, -30, 0, 30, 60, 90] # Set latitude ticks
colorbar_location: bottom
extent: null # If defined, restrict the projection to a region. Format [lon1, lon2,
→ lat1, lat2]
suptitle_pos: 0.87 # Title position in the figure.
```

Each entry in variables corresponds to a variable definition. Use the default entry to apply generic options to all variables. Example:

```
variables:
  # Define default. Variable definitions completely override the default
  # not just the values defined. If you want to override only the defined
  # values, use yaml anchors as shown
  default: &default
      colors: RdYlBu_r # Matplotlib colormap to use for the colorbar
     N: 20 # Number of map intervals to plot
     bad: [0.9, 0.9, 0.9] # Color to use when no data
  pr:
      <c: *default
     colors: gist_earth_r
      # Define bounds of the colorbar, as a list of
     bounds: 0-10.5,0.5 # Set colorbar bounds, as a list or in the format min-max,
→interval
      extend: max # Set extend parameter of mpl colorbar. See https://matplotlib.org/
⇔stable/api/_as_gen/matplotlib.pyplot.colorbar.html
  SOS:
      # If default is defined, entries are treated as map specific option.
      # Missing values in map definitionas are taken from variable's default
      # definition
      default:
         <c: *default
         bounds: 25-41,1
         extend: both
      arctic:
         bounds: 25-40,1
      antarctic:
         bounds: 30-40,0.5
  nao: &nao
     <c: *default
      extend: both
      # Variable definitions can override map parameters. Use with caution.
     bounds: [-0.03, -0.025, -0.02, -0.015, -0.01, -0.005, 0., 0.005, 0.01, 0.015, 0.02,
\leftrightarrow 0.025, 0.03]
     projection: PlateCarree
      smooth: true
     lon: [-90, -60, -30, 0, 30]
      lat: [20, 40, 60, 80]
      colorbar_location: bottom
      suptitle_pos: 0.87
  sam:
      <<: *nao
```

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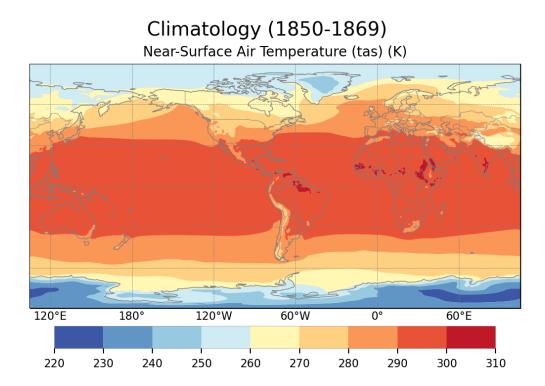
(continued from previous page)

```
lat: [-90, -80, -70, -60, -50]
projection: SouthPolarStereo
projection_kwargs:
    central_longitude: 270
smooth: true
lon: [-120, -60, 0, 60, 120, 180]
```

## 14.2.4 Variables

Any, but the variables' number of dimensions should match the ones expected by each plot.

# 14.2.5 Example plots



Global climatology of tas.

Seasonal climatology of pr, with a custom colorbar.

Monthly climatology of sivol, only for March and September.

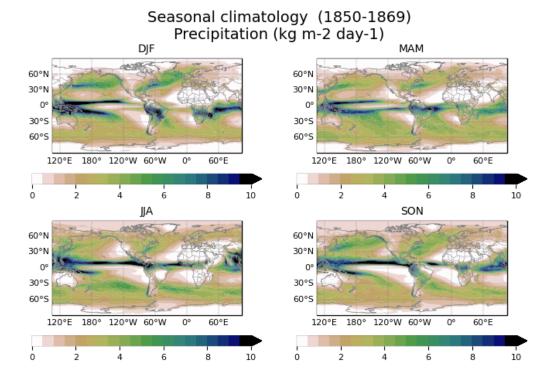
Timeseries of Niño 3.4 index, computed directly with the preprocessor.

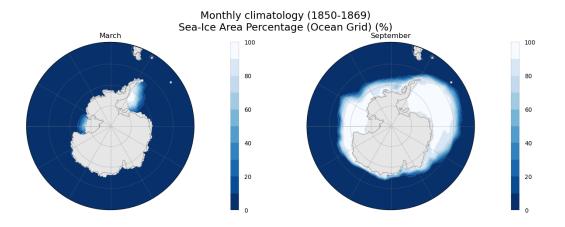
Annual cycle of tas.

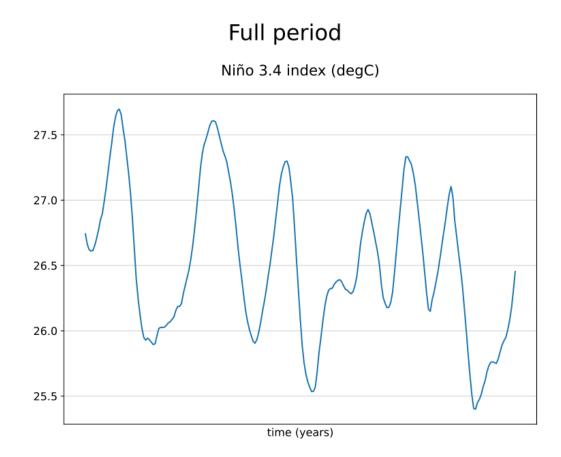
Timeseries of tas including a reference dataset.

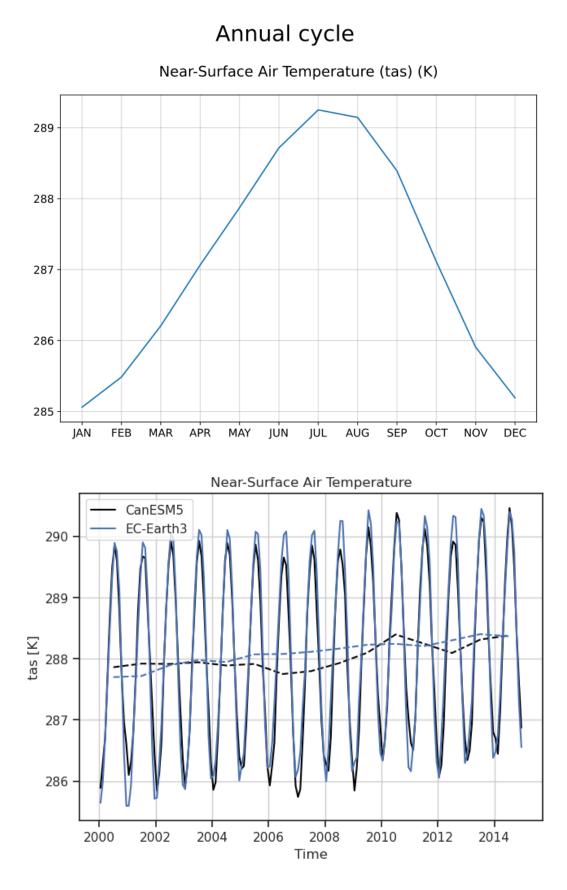
Annual cycle of tas including a reference dataset.

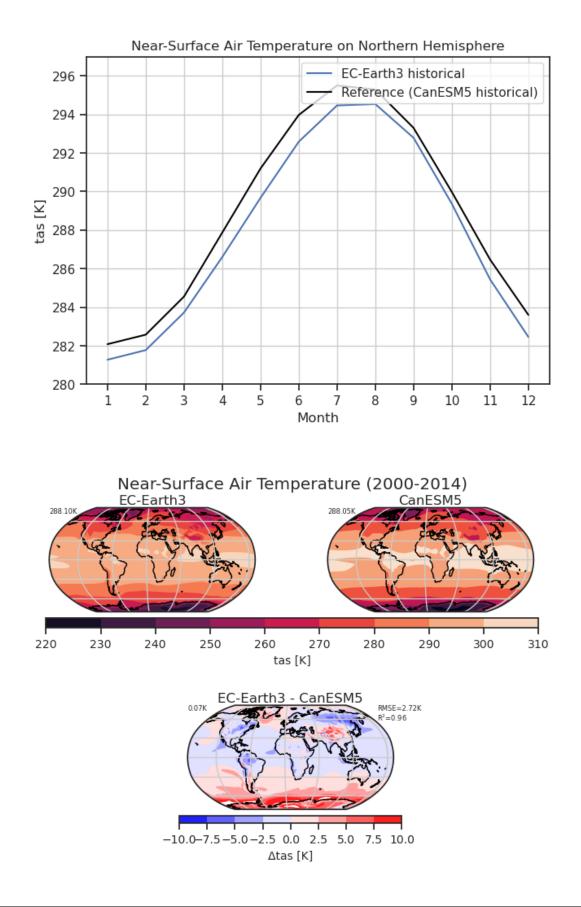
Global climatology of tas including a reference dataset.

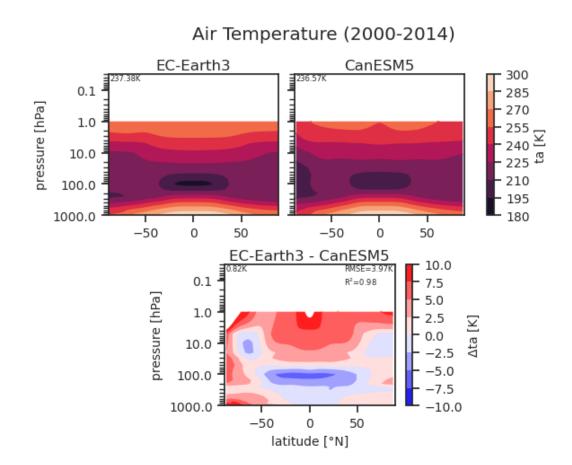












Zonal mean profile of ta including a reference dataset.

1D profile of ta including a reference dataset.

Zonal mean pr including a reference dataset.

Hovmoeller plot (pressure vs. time) of ta including a reference dataset.

Hovmoeller plot (time vs. latitude) of tas including a reference dataset

# **14.3 Psyplot Diagnostics**

# 14.3.1 Overview

These recipes showcase the use of the Psyplot diagnostic that provides a high-level interface to Psyplot for ESMValTool recipes.

# 14.3.2 Available recipes and diagnostics

Recipes are stored in recipes/

recipe\_psyplot.yml

Diagnostics are stored in diag\_scripts/

• psyplot\_diag.py

# 14.3.3 Variables

Arbitrary variables are supported.

# 14.3.4 Observations and reformat scripts

Arbitrary datasets are supported.

# 14.3.5 References

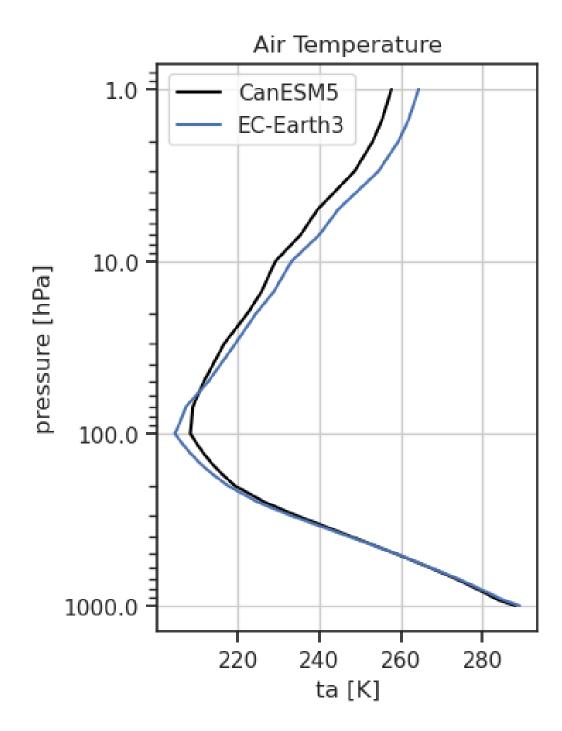
• Sommer, (2017), The psyplot interactive visualization framework, Journal of Open Source Software, 2(16), 363, doi:10.21105/joss.00363

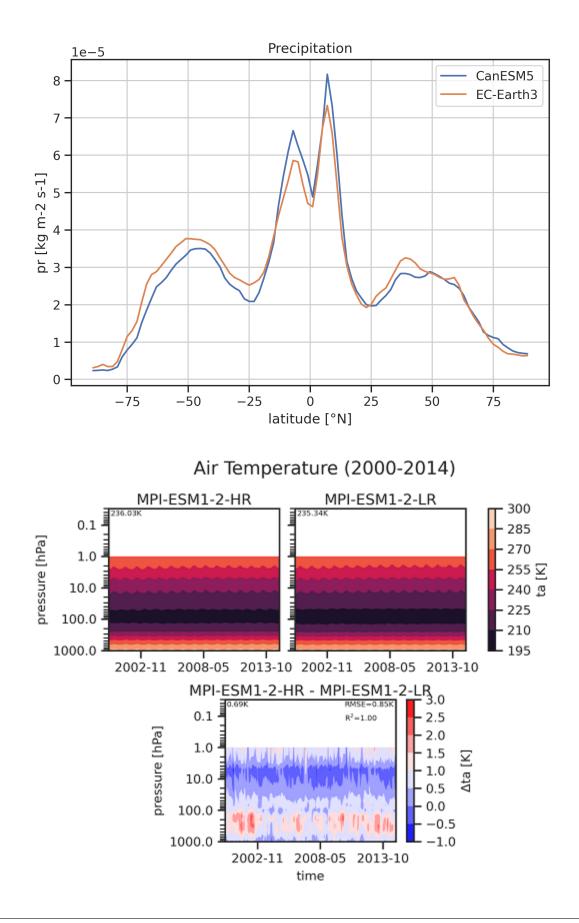
# 14.3.6 Example plots

# **14.4 Seaborn Diagnostics**

# 14.4.1 Overview

These recipes showcase the use of the Seaborn diagnostic that provides a high-level interface to Seaborn for ESMVal-Tool recipes.





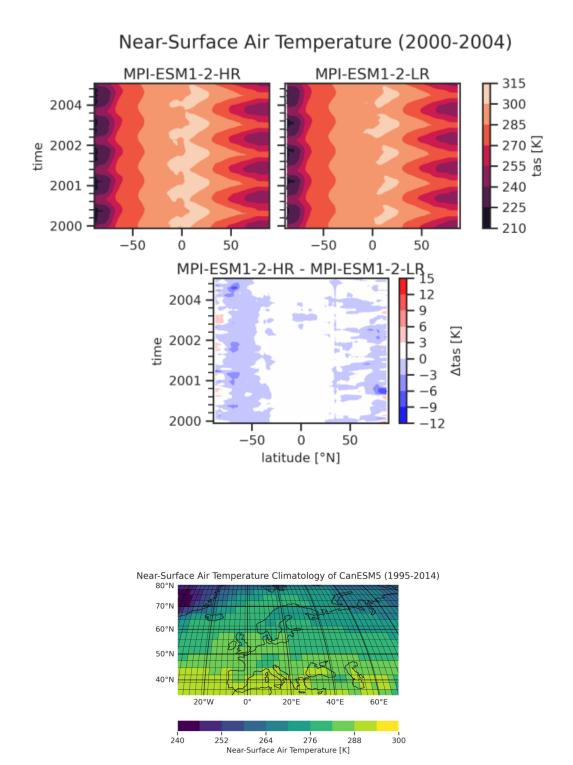
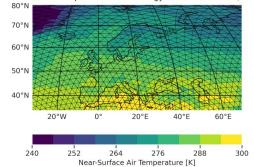


Fig. 1: Historical near-surface air temperature climatology over Europe simulated by CanESM5 between 1995 and 2014. The plot visualizes the invidividual rectangular grid cells of the model's regular grid.



Near-Surface Air Temperature Climatology of ICON-ESM-LR (1995-2014)

Fig. 2: Historical near-surface air temperature climatology over Europe simulated by ICON-ESM-LR between 1995 and 2014. The plot visualizes the invidividual triangular grid cells of the model's unstructured grid.

# 14.4.2 Available recipes and diagnostics

Recipes are stored in recipes/

• recipe\_seaborn.yml

Diagnostics are stored in diag\_scripts/

• seaborn\_diag.py

# 14.4.3 Variables

Arbitrary variables are supported.

# 14.4.4 Observations and reformat scripts

Arbitrary datasets are supported.

# 14.4.5 References

• Waskom, M. L. (2021), seaborn: statistical data visualization, Journal of Open Source Software, 6(60), 3021, doi:10.21105/joss.03021.

# 14.4.6 Example plots

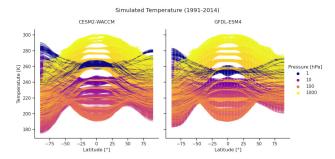


Fig. 3: Monthly and zonal mean temperatures vs. latitude in the period 1991-2014 for two Earth system models (CESM2-WACCM and GFDL-ESM4). Colors visualize the corresponding pressure levels.

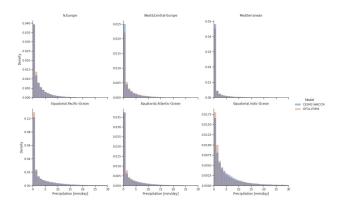


Fig. 4: Spatiotemporal distribution of daily precipitation in the period 2005-2014 for six IPCC AR6 regions simulated by two Earth system models (CESM2-WACCM and GFDL-ESM4). Each day in each grid cell in the corresponding regions is considered with equal weight.

## CHAPTER

# FIFTEEN

# **ATMOSPHERE**

# 15.1 Blocking metrics and indices, teleconnections and weather regimes (MiLES)

### 15.1.1 Overview

Atmospheric blocking is a recurrent mid-latitude weather pattern identified by a large-amplitude, quasi-stationary, long-lasting, high-pressure anomaly that "blocks" the westerly flow forcing the jet stream to split or meander (Rex, 1950).

It is typically initiated by the breaking of a Rossby wave in a diffluence region at the exit of the storm track, where it amplifies the underlying stationary ridge (Tibaldi and Molteni, 1990). Blocking occurs more frequently in the Northern Hemisphere cold season, with larger frequencies observed over the Euro-Atlantic and North Pacific sectors. Its lifetime oscillates from a few days up to several weeks (Davini et al., 2012) sometimes leading to winter cold spells or summer heat waves.

To this end, the MId-Latitude Evaluation System (MiLES) was developed as stand-alone package (https://github.com/ oloapinivad/MiLES) to support analysis of mid-latitude weather patterns in terms of atmospheric blocking, teleconnections and weather regimes. The package was then implemented as recipe for ESMValTool.

The tool works on daily 500hPa geopotential height data (with data interpolated on a common 2.5x2.5 grid) and calculates the following diagnostics:

#### **1D Atmospheric Blocking**

Tibaldi and Molteni (1990) index for Northern Hemisphere. Computed at fixed latitude of 60N, with delta of -5,-2.5,0,2.5,5 deg, fiN=80N and fiS=40N. Full timeseries and climatologies are provided in NetCDF4 Zip format.

#### **2D Atmospheric blocking**

Following the index by Davini et al. (2012). It is a 2D version of Tibaldi and Molteni (1990) for Northern Hemisphere atmospheric blocking evaluating meridional gradient reversal at 500hPa. It computes both Instantaneous Blocking and Blocking Events frequency, where the latter allows the estimation of the each blocking duration. It includes also two blocking intensity indices, i.e. the Meridional Gradient Index and the Blocking Intensity index. In addition the orientation (i.e. cyclonic or anticyclonic) of the Rossby wave breaking is computed. A supplementary Instantaneous Blocking index with the GHGS2 condition (see Davini et al., 2012) is also evaluated. Full timeseries and climatologies are provided in NetCDF4 Zip format.

#### **Z500 Empirical Orthogonal Functions**

Based on SVD. The first 4 EOFs for North Atlantic (over the 90W-40E 20N-85N box) and Northern Hemisphere (20N-85N) or a custom region are computed. North Atlantic Oscillation, East Atlantic Pattern, and Arctic Oscillation can be evaluated. Figures showing linear regression of PCs on monthly Z500 are provided. PCs and eigenvectors, as well as the variances explained are provided in NetCDF4 Zip format.

#### **North Atlantic Weather Regimes**

Following k-means clustering of 500hPa geopotential height. 4 weather regimes over North Atlantic (80W-40E 30N-87.5N) are evaluated using anomalies from daily seasonal cycle. This is done retaining the first North Atlantic EOFs which explains the 80% of the variance to reduce the phase-space dimensions and then applying k-means clustering using Hartigan-Wong algorithm with k=4. Figures report patterns and frequencies of occurrence. NetCDF4 Zip data are saved. Only 4 regimes and DJF supported so far.

# 15.1.2 Available recipes and diagnostics

Recipes are stored in recipes/

- recipe\_miles\_block.yml
- recipe\_miles\_eof.yml
- recipe\_miles\_regimes.yml

Diagnostics are stored in diag\_scripts/miles/

- miles\_block.R
- miles\_eof.R
- miles\_regimes.R

and subroutines

- basis\_functions.R
- block\_figures.R
- eof\_figures.R
- regimes\_figures.R
- block\_fast.R
- eof\_fast.R
- miles\_parameters.R
- regimes\_fast.R

miles\_parameters.R contains additional internal parameters which affect plot sizes, colortables etc.

# 15.1.3 User settings

1. miles\_block.R

Required settings for variables

- reference\_dataset: reference dataset for comparison
- reference\_exp: optional reference experiment for comparison (to use when comparing two experiments of the same dataset)

Required settings for script

- seasons: Selected season('DJF','MAM','JJA','SON','ALL') or your period as e.g. 'Jan\_Feb\_Mar'
- 2. miles\_eof.R

Required settings for variables

- reference\_dataset: reference dataset for comparison
- reference\_exp: optional reference experiment for comparison (to use when comparing two experiments of the same dataset)

Required settings for script

- seasons: Selected season('DJF','MAM','JJA','SON','ALL') or your period as e.g. 'Jan\_Feb\_Mar'
- teles: Select EOFs ('NAO','AO','PNA') or specify custom area as "lon1\_lon2\_lat1\_lat2"
- 3. miles\_regimes.R

Required settings for variables

- reference\_dataset: reference dataset
- reference\_exp: optional reference experiment for comparison (to use when comparing two experiments of the same dataset)

Required or optional settings for script

• None (the two parameters seasons and nclusters in the recipe should not be changed)

# 15.1.4 Variables

• zg (atmos, daily mean, longitude latitude time)

# 15.1.5 Observations and reformat scripts

• ERA-INTERIM

# 15.1.6 References

- REX, D. F. (1950), Blocking Action in the Middle Troposphere and its Effect upon Regional Climate. Tellus, 2: 196-211. doi: http://doi.org/10.1111/j.2153-3490.1950.tb00331.x
- Davini, P., C. Cagnazzo, S. Gualdi, and A. Navarra (2012): Bidimensional Diagnostics, Variability, and Trends of Northern Hemisphere Blocking. J. Climate, 25, 6496–6509, doi: http://doi.org/10.1175/JCLI-D-12-00032.1.
- Tibaldi S, Molteni F.: On the operational predictability of blocking. Tellus A 42(3): 343–365, doi: 10.1034/j.1600-0870.1990.t01-2-00003.x, 1990. https://doi.org/10.1034/j.1600-0870.1990.t01-2-00003.x
- Paolo Davini. (2018, April 30). MiLES Mid Latitude Evaluation System (Version v0.51). Zenodo. http://doi.org/10.5281/zenodo.1237838

# 15.1.7 Example plots

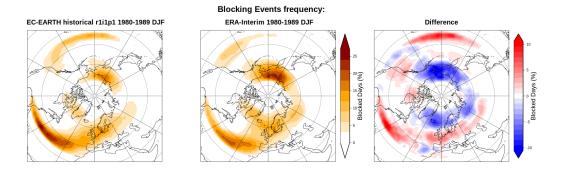


Fig. 1: Blocking Events frequency for a CMIP5 EC-Earth historical run (DJF 1980-1989), compared to ERA-Interim. Units are percentage of blocked days per season.

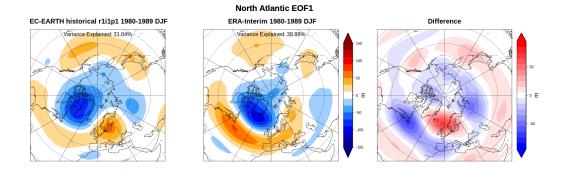


Fig. 2: North Atlantic Oscillation for a CMIP5 EC-Earth historical run (DJF 1980-1989) compared to ERA-Interim, shown as the linear regression of the monthly Z500 against the first Principal Component (PC1) of the North Atlantic region.

# 15.2 Clouds

# 15.2.1 Overview

Four recipes are available to evaluate cloud climatologies from CMIP models.

- 1) recipe\_clouds\_bias.yml computes climatologies and creates map plots of multi-model mean, mean bias, absolute bias and relative bias of a given variable. Similar to IPCC AR5 (ch. 9) fig. 9.2 a/b/c (Flato et al., 2013).
- 2) recipe\_clouds\_ipcc.yml computes multi-model mean bias and zonal means of the clouds radiative effect (short-wave, longwave and net). Similar to IPCC AR5 (ch. 9) fig. 9.5 (Flato et al., 2013).
- 3) Recipe recipe\_lauer13jclim.yml computes the climatology and interannual variability of climate relevant cloud variables such as cloud radiative forcing (CRE), liquid water path (lwp), cloud amount (clt), and total precipitation (pr) reproducing some of the evaluation results of Lauer and Hamilton (2013). The recipe includes a comparison of the geographical distribution of multi-year average cloud parameters from individual models and the multi-model mean with satellite observations. Taylor diagrams are generated that show the multi-year annual or seasonal average performance of individual models and the multi-model mean in reproducing satellite observations. The diagnostic also facilitates the assessment of the bias of the multi-model mean and zonal averages of individual models compared with satellite observations. Interannual variability is estimated as the relative temporal standard deviation from multi-year timeseries of data with the temporal standard deviations calculated from monthly anomalies after subtracting the climatological mean seasonal cycle. Note that the satellite observations used in the original recipe (UWisc) is not maintained anymore and has been superseeded by MAC-LWP (Elsaesser et al., 2017). We recommend using MAC-LWP.
- 4) Recipe family recipe\_lauer22jclim\_\*.yml is an extension of recipe\_lauer13jclim.yml for evaluation of cloud radiative forcing (CRE), liquid water path (lwp), ice water path (clivi), total cloud amount (clt), cloud liquid water content (clw), cloud ice water content (cli), cloud fraction (cl) and water vapor path (prw) from CMIP6 models in comparison to CMIP5 results and satellite observations. Wherever possible, the diagnostics use multi-observational products as reference datasets. The recipe family reproduces all figures from Lauer et al. (2023): maps of the geographical distribution of multi-year averages, Taylor diagrams for multi-year annual averages, temporal variability, seasonal cycle amplitude, cloud ice fraction as a function of temperature, zonal means of 3-dim cloud liquid/ice content and cloud fraction, matrices of cloud cover and total cloud water path as a function of SST and 500 hPa vertical velocity, shortwave CRE and total cloud water path binned by total cloud cover and pdfs of total cloud cover for selected regions.

# 15.2.2 Available recipes and diagnostics

Recipes are stored in recipes/clouds

- recipe\_clouds\_bias.yml
- recipe\_clouds\_ipcc.yml
- recipe\_lauer13jclim.yml
- recipe\_lauer22jclim\_\*.yml (\* = fig1\_clim\_amip, fig1\_clim, fig2\_taylor\_amip, fig2\_taylor, fig3-4\_zonal, fig5\_lifrac, fig6\_interannual, fig7\_seas, fig8\_dyn, fig9-11ab\_scatter, fig9-11c\_pdf)

Diagnostics are stored in diag\_scripts/clouds/

- clouds.ncl: global maps of (multi-year) annual means including multi-model mean
- clouds\_bias.ncl: global maps of the multi-model mean and the multi-model mean bias
- clouds\_dyn\_matrix.ncl: cloud properties by dynamical regime (SST, omega500)
- clouds\_interannual.ncl: global maps of the interannual variability

- clouds\_ipcc.ncl: global maps of multi-model mean minus observations + zonal averages of individual models, multi-model mean and observations
- clouds\_lifrac\_scatter.ncl: cloud liquid water fraction as a function of temperature
- clouds\_lifrac\_scatter\_postproc.ncl: additional plots and diagnostics using the output of clouds\_lifrac\_scatter.ncl for given CMIP5/CMIP6 model pairs
- clouds\_pdf.ncl: pdf of cloud parameters
- clouds\_seasonal\_cycle.ncl: seasonal cycle amplitude
- clouds\_taylor.ncl: Taylor diagrams as in Lauer and Hamilton (2013)
- clouds\_taylor\_double.ncl: Taylor diagrams as in Lauer et al. (2023)
- clouds\_zonal.ncl: zonal means of 3-dim variables

# 15.2.3 User settings in recipe

1. Script clouds.ncl

Required settings (scripts)

none

- embracesetup: true = 2 plots per line, false = 4 plots per line (default)
- explicit\_cn\_levels: explicit contour levels (array)
- extralegend: plot legend(s) to extra file(s)
- filename\_add: optionally add this string to plot filesnames
- multiobs\_exclude: list of *observational* datasets to be excluded when calculating uncertainty estimates from multiple observational datasets (see also multiobs\_uncertainty)
- multiobs\_uncertainty: calculate uncertainty estimates from multiple observational datasets (true, false); by default, all "obs", "obs6", "obs4mips" and "native6" datasets are used; any of such datasets can be explicitly excluded when also specifying "multiobs\_exclude"
- panel\_labels: label individual panels (true, false)
- PanelTop: manual override for "@gnsPanelTop" used by panel plot(s)
- projection: map projection for plotting (default = "CylindricalEquidistant")
- showdiff: calculate and plot differences model reference (default = false)
- showyears: add start and end years to the plot titles (default = false)
- rel\_diff: if showdiff = true, then plot relative differences (%) (default = False)
- ref\_diff\_min: lower cutoff value in case of calculating relative differences (in units of input variable)
- region: show only selected geographic region given as latmin, latmax, lonmin, lonmax
- timemean: time averaging "seasonal" = DJF, MAM, JJA, SON), "annual" = annual mean
- treat\_var\_as\_error: treat variable as error when averaging (true, false); true: avg = sqrt(mean(var\*var)), false: avg = mean(var)
- var: short\_name of variable to process (default = "" use first variable in variable list)

none

Optional settings (variables)

- long\_name: variable description
- reference\_dataset: reference dataset; REQUIRED when calculating differences (showdiff = True)
- units: variable units (for labeling plot only)

#### Color tables

- variable "lwp": diag\_scripts/shared/plot/rgb/qcm3.rgb
- 2. Script clouds\_bias.ncl

Required settings (scripts)

#### none

Optional settings (scripts)

- plot\_abs\_diff: additionally also plot absolute differences (true, false)
- plot\_rel\_diff: additionally also plot relative differences (true, false)
- projection: map projection, e.g., Mollweide, Mercator
- timemean: time averaging, i.e. "seasonalclim" (DJF, MAM, JJA, SON), "annualclim" (annual mean)
- Required settings (variables)\*
- reference\_dataset: name of reference datatset

#### **Optional settings (variables)**

• long\_name: description of variable

#### Color tables

- variable "tas": diag\_scripts/shared/plot/rgb/ipcc-tas.rgb, diag\_scripts/shared/plot/rgb/ipcc-tas-delta.rgb
- variable "pr-mmday": diag\_scripts/shared/plots/rgb/ipcc-precip.rgb, diag\_scripts/shared/plot/rgb/ipcc-precip-delta.rgb
- 3. Script clouds\_dyn\_matrix.ncl

#### Required settings (scripts)

- var\_x: short name of variable on x-axis
- var\_y: short name of variable on y-axis
- var\_z: short name of variable to be binned
- xmin: min x value for generating x bins
- xmax: max x value for generating x bins
- ymin: min y value for generating y bins
- ymax: max y value for generating y bins

- clevels: explicit values for probability labelbar (array)
- filename\_add: optionally add this string to plot filesnames

- nbins: number of equally spaced bins (var\_x), default = 100
- sidepanels: show/hide side panels (default = False)
- xlabel: label overriding variable name for x-axis (e.g. SST)
- ylabel: label overriding variable name for y-axis (e.g. omega500)
- zdmin: min z value for labelbar (difference plots)
- zdmax: max z value for labelbar (difference plots)
- zmin: min z value for labelbar
- zmax: max z value for labelbar

#### Optional settings (variables)

- reference\_dataset: reference dataset
- 4. Script clouds\_interannual.ncl

Required settings (scripts)

#### none

Optional settings (scripts)

- colormap: e.g., WhiteBlueGreenYellowRed, rainbow
- epsilon: "epsilon" value to be replaced with missing values
- explicit\_cn\_levels: use these contour levels for plotting
- filename\_add: optionally add this string to plot filesnames
- projection: map projection, e.g., Mollweide, Mercator
- var: short\_name of variable to process (default = "" use first variable in variable list)

Required settings (variables)

none

Optional settings (variables)

- long\_name: description of variable
- reference\_dataset: name of reference datatset
- 5. Script clouds\_ipcc.ncl

Required settings (scripts)

none

- explicit\_cn\_levels: contour levels
- highlight\_dataset: name of dataset to highlight (default = "MultiModelMean")
- mask\_ts\_sea\_ice: true = mask T < 272 K as sea ice (only for variable "ts"); false = no additional grid cells masked for variable "ts"
- projection: map projection, e.g., Mollweide, Mercator
- styleset: style set for zonal mean plot ("CMIP5", "DEFAULT")

- timemean: time averaging, i.e. "seasonalclim" (DJF, MAM, JJA, SON), "annualclim" (annual mean)
- valid\_fraction: used for creating sea ice mask (mask\_ts\_sea\_ice = true): fraction of valid time steps required to mask grid cell as valid data

• reference\_dataset: name of reference data set

Optional settings (variables)

- long\_name: description of variable
- units: variable units

#### Color tables

- variables "pr", "pr-mmday": diag\_scripts/shared/plot/rgb/ipcc-precip-delta.rgb
- 6. Script clouds\_lifrac\_scatter.ncl

Required settings (scripts)

none

Optional settings (scripts)

- · filename\_add: optionally add this string to plot filesnames
- min\_mass: minimum cloud condensate (same units as clw, cli)
- mm\_mean\_median: calculate multi-model mean and meadian
- nbins: number of equally spaced bins (ta (x-axis)), default = 20
- panel\_labels: label individual panels (true, false)
- PanelTop: manual override for "@gnsPanelTop" used by panel plot(s)s

*Required settings (variables)* 

Optional settings (variables)

- reference\_dataset: reference dataset
- 7. Script clouds\_lifrac\_scatter\_postproc.ncl

Required settings (scripts)

- models: array of CMIP5/CMIP6 model pairs to be compared
- refname: name of reference dataset

Optional settings (scripts)

- nbins: number of bins used by clouds\_lifrac\_scatter.ncl (default = 20)
- reg: region (string) (default = "")
- t\_int: array of temperatures for printing additional diagnostics

Required settings (variables)

none

```
Optional settings (variables)
```

none

- 8. Script clouds\_pdf.ncl
  - Required settings (scripts)
    - xmin: min value for bins (x axis)
    - xmax: max value for bins (y axis)

Optional settings (scripts)

- filename\_add: optionally add this string to output filenames
- plot\_average: show average frequency per bin
- · region: show only selected geographic region given as latmin, latmax, lonmin, lonmax
- styleset: "CMIP5", "DEFAULT"
- ymin: min value for frequencies (%) (y axis)
- ymax: max value for frequencies (%) (y axis)

Required settings (variables)

- Optional settings (variables)
  - reference\_dataset: reference dataset
- 9. Script clouds\_seasonal\_cycle.ncl

Required settings (scripts)

none

**Optional settings** (scripts)

- colormap: e.g., WhiteBlueGreenYellowRed, rainbow
- epsilon: "epsilon" value to be replaced with missing values
- explicit\_cn\_levels: use these contour levels for plotting
- · filename\_add: optionally add this string to plot filesnames
- projection: map projection, e.g., Mollweide, Mercator
- showyears: add start and end years to the plot titles (default = false)
- var: short\_name of variable to process (default = "" i.e. use first variable in variable list)

Required settings (variables)

#### Optional settings (variables)

- long\_name: description of variable
- reference\_dataset: name of reference dataset
- 10. Script clouds\_taylor.ncl

Required settings (scripts)

none

#### Optional settings (scripts)

• embracelegend: false (default) = include legend in plot, max. 2 columns with dataset names in legend; true = write extra file with legend, max. 7 dataset names per column in legend, alternative observational dataset(s) will be plotted as a red star and labeled "altern. ref. dataset" in legend (only if dataset is of class "OBS")

- estimate\_obs\_uncertainty: true = estimate observational uncertainties from mean values (assuming fractions of obs. RMSE from documentation of the obs data); only available for "CERES-EBAF", "MODIS", "MODIS-L3"; false = do not estimate obs. uncertainties from mean values
- filename\_add: legacy feature: arbitrary string to be added to all filenames of plots and netcdf output produced (default = "")
- legend\_filter: do not show individual datasets in legend that are of project "legend\_filter" (default = "")
- mask\_ts\_sea\_ice: true = mask T < 272 K as sea ice (only for variable "ts"); false = no additional grid cells masked for variable "ts"
- multiobs\_exclude: list of *observational* datasets to be excluded when calculating uncertainty estimates from multiple observational datasets (see also multiobs\_uncertainty)
- multiobs\_uncertainty: calculate uncertainty estimates from multiple observational datasets (true, false); by default, all "obs", "obs6", "obs4mips" and "native6" datasets are used; any of such datasets can be explicitly excluded when also specifying "multiobs\_exclude"
- styleset: "CMIP5", "DEFAULT" (if not set, clouds\_taylor.ncl will create a color table and symbols for plotting)
- timemean: time averaging; annualclim (default) = 1 plot annual mean; seasonalclim = 4 plots (DJF, MAM, JJA, SON)
- valid\_fraction: used for creating sea ice mask (mask\_ts\_sea\_ice = true): fraction of valid time steps required to mask grid cell as valid data
- var: short\_name of variable to process (default = "" use first variable in variable list)

• reference\_dataset: name of reference data set

*Optional settings (variables)* 

none

11. Script clouds\_taylor\_double.ncl

Required settings (scripts)

none

- filename\_add: legacy feature: arbitrary string to be added to all filenames of plots and netcdf output produced (default = "")
- multiobs\_exclude: list of *observational* datasets to be excluded when calculating uncertainty estimates from multiple observational datasets (see also multiobs\_uncertainty)
- multiobs\_uncertainty: calculate uncertainty estimates from multiple observational datasets (true, false); by default, all "obs", "obs6", "obs4mips" and "native6" datasets are used; any of such datasets can be explicitely excluded when also specifying "multiobs\_exclude"
- projectcolors: colors for each projectgroups (e.g. (/"(/0.0, 0.0, 1.0/)", "(/1.0, 0.0, 0.0/)"/)
- projectgroups: calculated mmm per "projectgroup" (e.g. (/"cmip5", "cmip6")/)
- styleset: "CMIP5", "DEFAULT" (if not set, CLOUDS\_TAYLOR\_DOUBLE will create a color table and symbols for plotting)
- timemean: time averaging; annualclim (default) = 1 plot annual mean, seasonalclim = 4 plots (DJF, MAM, JJA, SON)

• var: short\_name of variable to process (default = "" - use first variable in variable list)

Required settings (variables)

• reference\_dataset: name of reference data set

Optional settings (variables)

12. Script clouds\_zonal.ncl

Required settings (scripts)

none

Optional settings (scripts)

- embracesetup: True = 2 plots per line, False = 4 plots per line (default)
- explicit\_cn\_levels: explicit contour levels for mean values (array)
- explicit\_cn\_dlevels: explicit contour levels for differences (array)
- extralegend: plot legend(s) to extra file(s)
- · filename\_add: optionally add this string to plot filesnames
- panel\_labels: label individual panels (true, false)
- PanelTop: manual override for "@gnsPanelTop" used by panel plot(s)
- showdiff: calculate and plot differences (default = False)
- rel\_diff: if showdiff = True, then plot relative differences (%) (default = False)
- rel\_diff\_min: lower cutoff value in case of calculating relative differences (in units of input variable)
- t\_test: perform t-test when calculating differences (default = False)
- timemean: time averaging "seasonal" = DJF, MAM, JJA, SON), "annual" = annual mean
- units\_to: target units (automatic conversion)

Required settings (variables)

none

Optional settings (variables)

- long\_name: variable description
- reference\_dataset: reference dataset; REQUIRED when calculating differences (showdiff = True)
- units: variable units (for labeling plot only)

# 15.2.4 Variables

- cl (atmos, monthly mean, longitude latitude time)
- clcalipso (atmos, monthly mean, longitude latitude time)
- cli (atmos, monthly mean, longitude latitude time)
- clw (atmos, monthly mean, longitude latitude time)
- clwvi (atmos, monthly mean, longitude latitude time)
- clivi (atmos, monthly mean, longitude latitude time)
- clt (atmos, monthly mean, longitude latitude time)

- pr (atmos, monthly mean, longitude latitude time)
- prw (atmos, monthly mean, longitude latitude time)
- rlut, rlutcs (atmos, monthly mean, longitude latitude time)
- rsut, rsutcs (atmos, monthly mean, longitude latitude time)
- ta (atmos, monthly mean, longitude latitude time)
- wap (atmos, monthly mean, longitude latitude time)

### 15.2.5 Observations/realanyses

- CALIPSO-GOCCP
- CALIPSO-ICECLOUD
- CERES-EBAF
- CLARA-AVHRR
- CLOUDSAT-L2
- ERA5
- ERA-Interim
- ESACCI-CLOUD
- ESACCI-WATERVAPOUR
- GPCP-SG
- ISCCP-FH
- MAC-LWP
- MODIS
- PATMOS-x
- UWisc

# 15.2.6 References

- Flato, G., J. Marotzke, B. Abiodun, P. Braconnot, S.C. Chou, W. Collins, P. Cox, F. Driouech, S. Emori, V. Eyring, C. Forest, P. Gleckler, E. Guilyardi, C. Jakob, V. Kattsov, C. Reason and M. Rummukainen, 2013: Evaluation of Climate Models. In: Climate Change 2013: The Physical Science Basis. Contribution of Working Group I to the Fifth Assessment Report of the Intergovernmental Panel on Climate Change [Stocker, T.F., D. Qin, G.-K. Plattner, M. Tignor, S.K. Allen, J. Boschung, A. Nauels, Y. Xia, V. Bex and P.M. Midgley (eds.)]. Cambridge University Press, Cambridge, United Kingdom and New York, NY, USA.
- Lauer A., and K. Hamilton (2013), Simulating clouds with global climate models: A comparison of CMIP5 results with CMIP3 and satellite data, J. Clim., 26, 3823-3845, doi: 10.1175/JCLI-D-12-00451.1.
- Lauer, A., L. Bock, B. Hassler, M. Schröder, and M. Stengel, Cloud climatologies from global climate models a comparison of CMIP5 and CMIP6 models with satellite data, J. Climate, 36(2), doi: 10.1175/JCLI-D-22-0181.1, 2023.

# 15.2.7 Example plots

# 15.3 Evaluate water vapor short wave radiance absorption schemes of ESMs with the observations, including ESACCI data.

# 15.3.1 Overview

The recipe contains several diagnostics to use ESACCI water vapour data to evaluate CMIP models.

The diagnostic deangelisf3f4.py reproduces figures 3 and 4 from DeAngelis et al. (2015): See also doc/sphinx/source/recipes/recipe\_deangelis15nat.rst This paper compares models with different schemes for water vapor short wave radiance absorption with the observations. Schemes using pseudo-k-distributions with more than 20 exponential terms show the best results.

The diagnostic diag\_tropopause.py plots given variable at cold point tropopause height, here Specific Humidity (hus) is used. This will be calculated from the ESACCI water vapour data CDR-4, which are planed to consist of threedimensional vertically resolved monthly mean water vapour data (in ppmv) with spatial resolution of 100 km, covering the troposphere and lower stratosphere. The envisaged coverage is 2010-2014. The calculation of hus from water vapour in ppmv will be part of the cmorizer. Here, ERA-Interim data are used.

The diagnostic diag\_tropopause\_zonalmean.py plots zonal mean for given variable for all pressure levels between 250 and 1hPa and at cold point tropopause height. Here Specific Humidity (hus) is used. This will be calculated from the ESACCI water vapour data CDR-3, which are planed to contain the vertically resolved water vapour ECV in units of ppmv (volume mixing ratio) and will be provided as zonal monthly means on the SPARC Data Initiative latitude/pressure level grid (SPARC, 2017; Hegglin et al., 2013). It covers the vertical range between 250 hPa and 1 hPa, and the time period 1985 to the end of 2019. The calculation of hus from water vapour in ppmv will be part of the cmorizer. Here, ERA-Interim data are used.

# 15.3.2 Available recipes and diagnostics

Recipes are stored in recipes/

• recipe\_cmug\_h2o.yml

Diagnostics are stored in diag\_scripts/

- deangelis15nat/deangelisf3f4.py
- cmug\_h2o/diag\_tropopause.py
- cmug\_h2o/diag\_tropopause\_zonalmean.py

# 15.3.3 User settings in recipe

The recipe can be run with different CMIP5 and CMIP6 models.

deangelisf3f4.py: For each model, two experiments must be given: a pre industrial control run, and a scenario with 4 times  $CO_2$ . Possibly, 150 years should be given, but shorter time series work as well. Currently, HOAPS data are included as place holder for expected ESACCI-WV data, type CDR-2: Gridded monthly time series of TCWV in units of kg/m2 (corresponds to prw) that cover the global land and ocean areas with a spatial resolution of  $0.05^{\circ} / 0.5^{\circ}$  for the period July 2002 to December 2017.

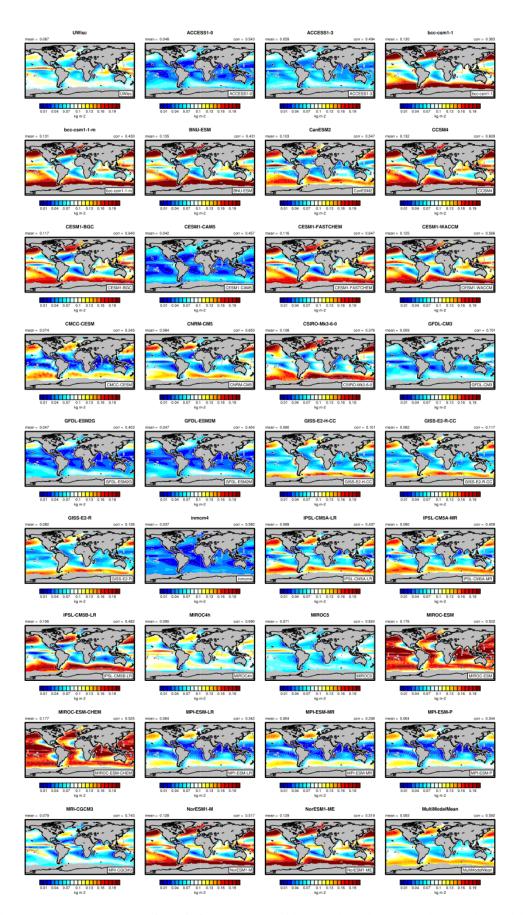


Fig. 3: The 20-yr average LWP (1986-2005) from the CMIP5 historical model runs and the multi-model mean in 1573 Evaluate water waper short wave radiance absorption schemes of ESMs with the O'Dell et al. 2008). Atomic water water state of the chinadology (1988-2007) based of SSMA, of ESMs with the O'Dell et al. 2008). Atomic water state of the chinadology (1988-2007) based of the state of t

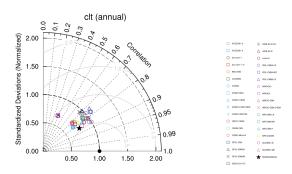


Fig. 4: Taylor diagram showing the 20-yr annual average performance of CMIP5 models for total cloud fraction as compared to MODIS satellite observations. Produced with recipe\_lauer13jclim.yml (diagnostic script clouds\_taylor.ncl).

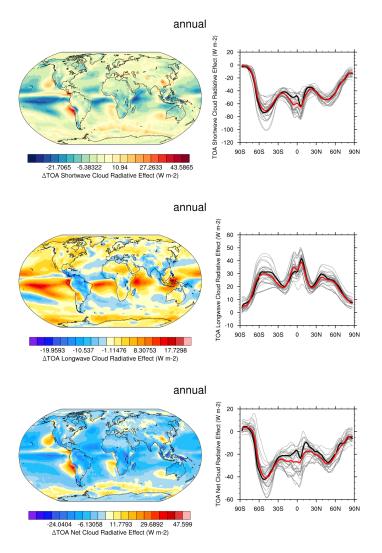


Fig. 5: 20-year average (1986-2005) annual mean cloud radiative effects of CMIP5 models against the CERES-EBAF (2001–2012). Top row shows the shortwave effect; middle row the longwave effect, and bottom row the net effect. Multi-model mean biases against CERES-EBAF are shown on the left, whereas the right panels show zonal averages from CERES-EBAF (thick black), the individual CMIP5 models (thin gray lines) and the multi-model mean (thick red line). Similar to Figure 9.5 of Flato et al., 2013. Produced with recipe\_clouds\_ipcc.yml (diagnostic script clouds\_ipcc.ncl).



Fig. 6: Interannual variability of modeled and observed (GPCP) precipitation rates estimated as relative tempo-15.3. Evaluate water vapor short (wave-radiance absorption schemes of ESMs with the alculated from rationality anomalies are calculated from posterior anomalies are calculated from estimatological mean seasonal cycle. Produced with recipe\_lauer13jclim.yml (clouds\_interannual.ncl).

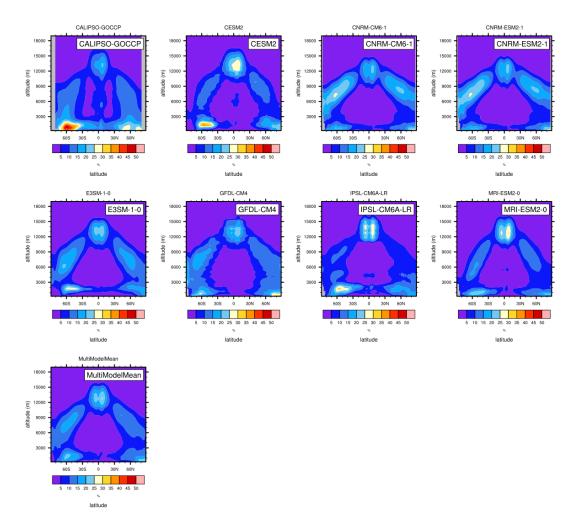


Fig. 7: Zonal mean of the multi-year annual mean cloud fraction as seen from CALIPSO from CMIP6 models in comparison to CALIPSO-GOCCP data. Produced with recipe\_lauer22jclim\_fig3-4\_zonal.yml (diagnostic script clouds\_zonal.ncl).

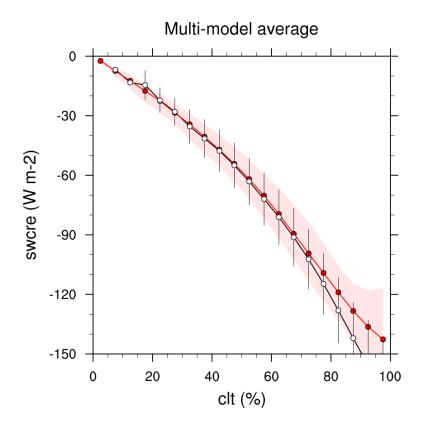


Fig. 8: Multi-year seasonal average (December-January-February) of cloud shortwave radiative effect (W  $m^{-2}$ ) vs. total cloud fraction (clt, %) averaged over the Southern Ocean defined as latitude belt 30°S-65°S (ocean grid cells only). Shown are the CMIP6 multi-model mean (red filled circles and lines) and observational estimates from ESACCI-CLOUD (black circles and lines). The red shaded areas represent the range between the 10th and 90th percentiles of the results from all individual models. Produced with recipe\_lauer22jclim\_fig9-11ab\_scatter.yml (diagnostic script clouds\_scatter.ncl).

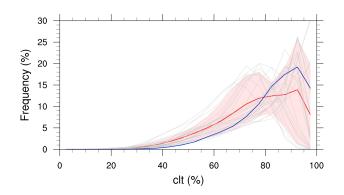


Fig. 9: Frequency distribution of monthly mean total cloud cover from CMIP6 models in comparison to ESACCI-CLOUD data. The red curve shows the multi-model average, the blue curve the ESACCI-CLOUD data and the thin gray lines the individual models. The red shading shows  $\pm 1$  standard deviation of the inter-model spread. Produced with recipe\_lauer22jclim\_fig9-11c\_pdf.yml (diagnostic script clouds\_pdf.ncl).

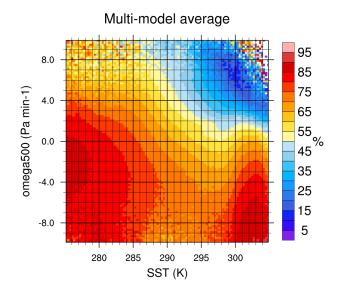


Fig. 10: 2-dimensional distribution of average total cloud cover (clt) binned by sea surface temperature (SST, x-axis) and vertical velocity at 500 hPa (<sub>500</sub>, y-axis) averaged over 20 years and all grid cells over the ocean. Produced with recipe\_lauer22jclim\_fig8\_dyn.yml (diagnostic script clouds\_dyn\_matrix.ncl).

#### 15.3.4 Variables

deangelisf3f4.py: \* *rsnstcs* (atmos, monthly, longitude, latitude, time) \* *rsnstcsnorm* (atmos, monthly, longitude, latitude, time) \* *prw* (atmos, monthly, longitude, latitude, time) \* *tas* (atmos, monthly, longitude, latitude, time)

diag\_tropopause.py: \* *hus* (atmos, monthly, longitude, latitude, time, plev) \* *ta* (atmos, monthly, longitude, latitude, time, plev)

diag\_tropopause\_zonalmean.py: \* *hus* (atmos, monthly, longitude, latitude, time, plev) \* *ta* (atmos, monthly, longitude, latitude, time, plev)

#### 15.3.5 Observations and reformat scripts

```
deangelisf3f4.py:
```

```
• rsnstcs:
CERES-EBAF
```

```
• prw
```

HOAPS, planed for ESACCI-WV data, type CDR-2

diag\_tropopause.py:

```
• hus
```

ERA-Interim, ESACCI water vapour paned

diag\_tropopause\_zonalmean.py:

- hus
- ERA-Interim, ESACCI water vapour paned

#### 15.3.6 References

 DeAngelis, A. M., Qu, X., Zelinka, M. D., and Hall, A.: An observational radiative constraint on hydrologic cycle intensification, Nature, 528, 249, 2015.

#### 15.3.7 Example plots

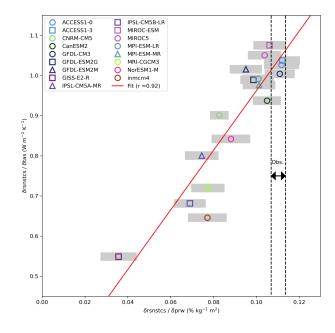


Fig. 11: Scatter plot and regression line computed between the ratio of the change of net short wave radiation (rsnst) and the change of the Water Vapor Path (prw) against the ratio of the change of netshort wave radiation for clear skye (rsnstcs) and the the change of surface temperature (tas). The width of horizontal shading for models and the vertical dashed lines for observations (Obs.) represent statistical uncertainties of the ratio, as the 95% confidence interval (CI) of the regression slope to the rsnst versus prw curve. For the prw observations ESACCI CDR-2 data from 2003 to 2014 are used.

## 15.4 Cloud Regime Error Metric (CREM)

#### 15.4.1 Overview

The radiative feedback from clouds remains the largest source of uncertainty in determining the climate sensitivity. Traditionally, cloud has been evaluated in terms of its impact on the mean top of atmosphere fluxes. However it is quite possible to achieve good performance on these criteria through compensating errors, with boundary layer clouds being too reflective but having insufficient horizontal coverage being a common example (e.g., Nam et al., 2012). Williams and Webb (2009) (WW09) propose a Cloud Regime Error Metric (CREM) which critically tests the ability of a model to simulate both the relative frequency of occurrence and the radiative properties correctly for a set of cloud regimes determined by the daily mean cloud top pressure, cloud albedo and fractional coverage at each grid-box. WW09 describe in detail how to calculate their metrics and we have included the CREMpd metric from their paper in ESMValTool, with clear references in the lodged code to tables in their paper. This has been applied to those CMIP5 models who have submitted the required diagnostics for their AMIP simulation (see Figure 8 below). As documented by WW09, a perfect score with respect to ISCCP would be zero. WW09 also compared MODIS/ERBE to ISCCP in order to provide an estimate of observational uncertainty. This was found to be 0.96 and this is marked on Figure 8,

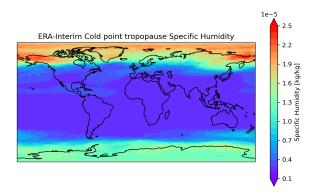


Fig. 12: Map of the average Specific Humidity (hus) at the cold point tropopause from ERA-Interim data. The diagnostic averages the complete time series, here 2010-2014.

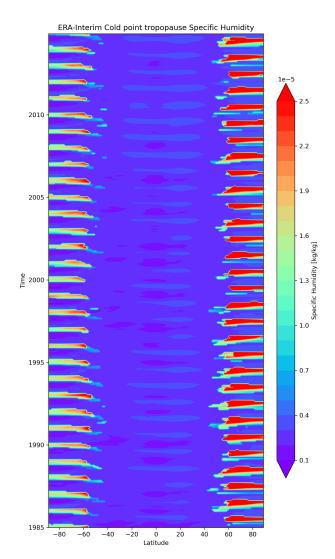


Fig. 13: Latitude versus time plot of the Specific Humidity (hus) at the cold point tropopause from ERA-Interim data.

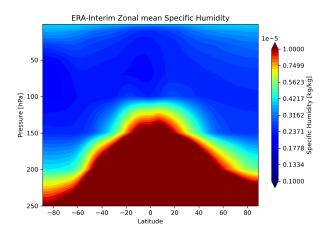


Fig. 14: Zonal average Specific Humidity (hus) between 250 and 1 hPa from ERA-Interim data. The diagnostic averages the complete time series, here 1985-2014.

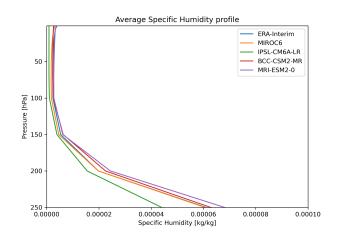


Fig. 15: Average Specific Humidity (hus) profile between 250 and 1 hPa from ERA-Interim and CMIP6 model data. The diagnostic averages the complete time series, here 1985-2014.

hence a model with a CREM similar to this value could be considered to have an error comparable with observational uncertainty, although it should be noted that this does not necessarily mean that the model lies within the observations for each regime. A limitation of the metric is that it requires a model to be good enough to simulate each regime. If a model is that poor that the simulated frequency of occurrence of a particular regime is zero, then a NaN will be returned from the code and a bar not plotted on the figure for that model.

The original publication recommends to use sea ice fields from one model also for other models that do not provide daily sea ice concentration. This is possible as sea ice concentrations are prescribed in the AMIP simulations and has been done to produce the example figure shown below.

#### 15.4.2 Available recipes and diagnostics

Recipes are stored in recipes/

• recipe\_williams09climdyn\_CREM.yml

Diagnostics are stored in diag\_scripts/crem/

• ww09\_esmvaltool.py

#### 15.4.3 User settings

None.

#### 15.4.4 Variables

- albisccp (atmos, daily mean, longitude latitude time)
- cltisccp (atmos, daily mean, longitude latitude time)
- pctisccp (atmos, daily mean, longitude latitude time)
- rlut (atmos, daily mean, longitude latitude time)
- rlutcs (atmos, daily mean, longitude latitude time)
- rsut (atmos, daily mean, longitude latitude time)
- rsutcs (atmos, daily mean, longitude latitude time)
- sic/siconc (seaice, daily mean, longitude latitude time)
- snc (atmos, daily mean, longitude latitude time)

If snc is not available then snw can be used instead. For AMIP simulations, sic/siconc is often not submitted as it a boundary condition and effectively the same for every model. In this case the same daily sic data set can be used for each model.

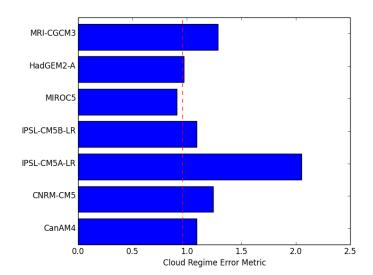
Note: in case of using sic/siconc data from a different model (AMIP), it has to be checked by the user that the calendar definitions of all data sets are compatible, in particular whether leap days are included or not.

#### 15.4.5 Observations and reformat scripts

All observational data have been pre-processed and included within the routine. These are ISCCP, ISCCP-FD, MODIS, ERBE. No additional observational data are required at runtime.

#### 15.4.6 References

- Nam, C., Bony, S., Dufresne, J.-L., and Chepfer, H.: The 'too few, too bright' tropical low-cloud problem in CMIP5 models, Geophys. Res. Lett., 39, L21801, doi: 10.1029/2012GL053421, 2012.
- Williams, K.D. and Webb, M.J.: A quantitative performance assessment of cloud regimes in climate models. Clim. Dyn. 33, 141-157, doi: 10.1007/s00382-008-0443-1, 2009.



#### 15.4.7 Example plots

Fig. 16: Cloud Regime Error Metrics (CREMpd) from William and Webb (2009) applied to selected CMIP5 AMIP simulations. A perfect score with respect to ISCCP is zero; the dashed red line is an indication of observational uncertainty. Note: as daily sea ice concentration (sic) is not available for all models shown, the regridded fields from CanAM4 have been used for all models.

# 15.5 Consecutive dry days

#### 15.5.1 Overview

Meteorological drought can in its simplest form be described by a lack of precipitation. First, a wet day threshold is set, which can be either a limit related to measurement accuracy, or more directly a process related to an amount that would break the drought. The diagnostic calculates the longest period of consecutive dry days, which is an indicator of the worst drought in the time series. Further, the diagnostic calculates the frequency of dry periods longer than a user defined number of days.

#### 15.5.2 Available recipes and diagnostics

Recipes are stored in recipes/

recipe\_consecdrydays.yml

Diagnostics are stored in diag\_scripts/droughtindex/

• diag\_cdd.py: calculates the longest period of consecutive dry days, and the frequency of dry day periods longer than a user defined length

#### 15.5.3 User settings in recipe

1. Script diag\_cdd.py

Required settings (script)

- plim: limit for a day to be considered dry [mm/day]
- frlim: the shortest number of consecutive dry days for entering statistic on frequency of dry periods.

Optional settings (script)

Under plot:

- cmap: the name of a colormap. cmocean colormaps are also supported.
- other keyword arguments to *esmvaltool.diag\_scripts.shared.plot.global\_pcolormesh()* can also be supplied.

#### 15.5.4 Variables

• pr (atmos, daily mean, time latitude longitude)

#### 15.5.5 Example plots

# 15.6 Evaluate water vapor short wave radiance absorption schemes of ESMs with the observations.

#### 15.6.1 Overview

The recipe reproduces figures from DeAngelis et al. (2015): Figure 1b to 4 from the main part as well as extended data figure 1 and 2. This paper compares models with different schemes for water vapor short wave radiance absorption with the observations. Schemes using pseudo-k-distributions with more than 20 exponential terms show the best results.

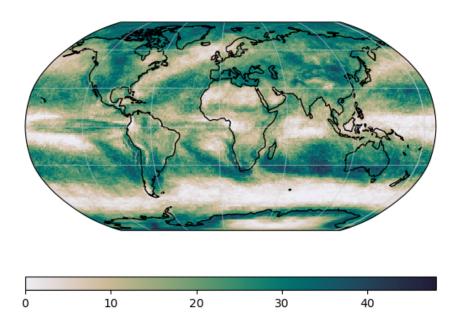


Fig. 17: Example of the number of occurrences with consecutive dry days of more than five days in the period 2001 to 2002 for the CMIP5 model bcc-csm1-1-m.

#### 15.6.2 Available recipes and diagnostics

Recipes are stored in recipes/

• recipe\_deangelis15nat.yml

Diagnostics are stored in diag\_scripts/

- deangelis15nat/deangelisf1b.py
- deangelis15nat/deangelisf2ext.py
- deangelis15nat/deangelisf3f4.py

#### 15.6.3 User settings in recipe

The recipe can be run with different CMIP5 and CMIP6 models. deangelisf1b.py: Several flux variables (W m<sup>-2</sup>) and up to 6 different model exeriements can be handeled. Each variable needs to be given for each model experiment. The same experiments must be given for all models. In DeAngelis et al. (2015) 150 year means are used but the recipe can handle any duration.

deangelisf2ext.py:

deangelisf3f4.py: For each model, two experiments must be given: a pre industrial control run, and a scenario with 4 times CO<sub>2</sub>. Possibly, 150 years should be given, but shorter time series work as well.

#### 15.6.4 Variables

deangelisf1b.py: Tested for:

- *rsnst* (atmos, monthly, longitude, latitude, time)
- *rlnst* (atmos, monthly, longitude, latitude, time)
- *lvp* (atmos, monthly, longitude, latitude, time)
- *hfss* (atmos, monthly, longitude, latitude, time)

any flux variable (W m<sup>-2</sup>) should be possible.

deangelisf2ext.py:

- *rsnst* (atmos, monthly, longitude, latitude, time)
- *rlnst* (atmos, monthly, longitude, latitude, time)
- *rsnstcs* (atmos, monthly, longitude, latitude, time)
- *rlnstcs* (atmos, monthly, longitude, latitude, time)
- *lvp* (atmos, monthly, longitude, latitude, time)
- *hfss* (atmos, monthly, longitude, latitude, time)
- tas (atmos, monthly, longitude, latitude, time)

deangelisf3f4.py: \* *rsnstcs* (atmos, monthly, longitude, latitude, time) \* *rsnstcsnorm* (atmos, monthly, longitude, latitude, time) \* *prw* (atmos, monthly, longitude, latitude, time) \* *tas* (atmos, monthly, longitude, latitude, time)

#### 15.6.5 Observations and reformat scripts

deangelisf1b.py: \* None

deangelisf2ext.py: \* None

deangelisf3f4.py:

- rsnstcs: CERES-EBAF
- prw

ERA-Interim, SSMI

#### 15.6.6 References

• DeAngelis, A. M., Qu, X., Zelinka, M. D., and Hall, A.: An observational radiative constraint on hydrologic cycle intensification, Nature, 528, 249, 2015.

#### 15.6.7 Example plots

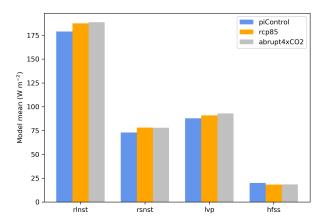


Fig. 18: Global average multi-model mean comparing different model experiments for the sum of upward long wave flux at TOA and net downward long wave flux at the surface (rlnst), heating from short wave absorption (rsnst), latent heat release from precipitation (lvp), and sensible heat flux (hfss). The panel shows three model experiments, namely the pre-industrial control simulation averaged over 150 years (blue), the RCP8.5 scenario averaged over 2091-2100 (orange) and the abrupt quadrupled CO<sub>2</sub> scenario averaged over the years 141-150 after CO<sub>2</sub> quadrupling in all models except CNRM-CM5-2 and IPSL-CM5A-MR, where the average is calculated over the years 131-140 (gray). The figure shows that energy sources and sinks readjust in reply to an increase in greenhouse gases, leading to a decrease in the sensible heat flux and an increase in the other fluxes.

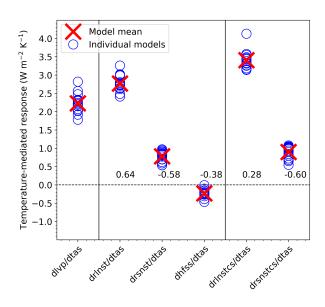


Fig. 19: The temperature-mediated response of each atmospheric energy budget term for each model as blue circles and the model mean as a red cross. The numbers above the abscissa are the cross-model correlations between dlvp/dtas and each other temperature-mediated response.'

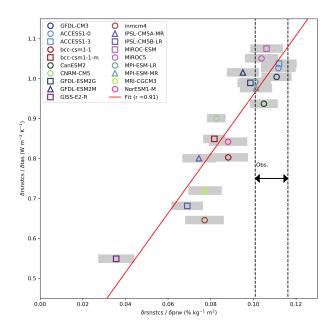


Fig. 20: Scatter plot and regression line the between the ratio of the change of net short wave radiation (rsnst) and the change of the Water Vapor Path (prw) against the ratio of the change of netshort wave radiation for clear skye (rsnstcs) and the the change of surface temperature (tas). The width of horizontal shading for models and the vertical dashed lines for observations (Obs.) represent statistical uncertainties of the ratio, as the 95% confidence interval (CI) of the regression slope to the rsnst versus prw curve. For the observations the minimum of the lower bounds of all CIs to the maximum of the upper bounds of all CIs is shown.

# 15.7 Diurnal temperature range

#### 15.7.1 Overview

The goal of this diagnostic is to compute a vulnerability indicator for the diurnal temperature range (DTR); the maximum variation in temperature within a period of 24 hours at a given location. This indicator was first proposed by the energy sector, to identify locations which may experience increased diurnal temperature variation in the future, which would put additional stress on the operational management of district heating systems. This indicator was defined as the DTR exceeding 5 degrees celsius at a given location and day of the year (Deandreis et al., N.D.). Projections of this indicator currently present high uncertainties, uncertainties associated to both Tmax and Tmin in future climate projections.

As well as being of use to the energy sector, the global-average DTR has been evaluated using both observations and climate model simulations (Braganza et. al., 2004) and changes in the mean and variability of the DTR have been shown to have a wide range of impacts on society, such as on the transmission of diseases (Lambrechts et al., 2011; Paaijmans et al., 2010).

The recipe recipe\_diurnal\_temperature\_index.yml computes first a mean DTR for a reference period using historical simulations and then, the number of days when the DTR from the future climate projections exceeds that of the reference period by 5 degrees or more. The user can define both the reference and projection periods, and the region to be considered. The output produced by this recipe consists of a four panel plot showing the maps of the projected mean DTR indicator for each season and a netcdf file containing the corresponding data.

## 15.7.2 Available recipes and diagnostics

Recipes are stored in recipes/

• recipe\_diurnal\_temperature\_index.yml

Diagnostics are stored in diag\_scripts/magic\_bsc/

• diurnal\_temp\_index.R : calculates the diaurnal temperature vulnerability index.

## 15.7.3 User settings

User setting files are stored in recipes/

1. recipe\_diurnal\_temperature\_index.yml

Required settings for script

• None

## 15.7.4 Variables

• tasmin and tasmax (atmos, daily, longitude, latitude, time)

#### 15.7.5 Observations and reformat scripts

None

#### 15.7.6 References

- Amiri, S. (2013). Economic and Environmental Benefits of CHP-based District Heating Systems in Sweden. Retrieved from http://www.sgc.se/ckfinder/userfiles/files/sokmotor/LiU67.pdf
- Braganza, K., Karoly, D. J., & Arblaster, J. M. (2004). Diurnal temperature range as an index of global climate change during the twentieth century. Geophysical Research Letters, 31(13), n/a n/a. https://doi.org/10.1029/2004GL019998
- Déandreis. C. (IPSL), Braconnot, P. (IPSL), and Planton, S.(CNRMGAME)(2014). Impact du changement climatique sur la gestion des réseaux de chaleur. DALKIA. access 24.02.2021. https://docplayer.fr/ Étude réalisée pour l'entreprise DALKIA. Last 9496504-Impact-du-changement-climatique-sur-la-gestion-des-reseaux-de-chaleur.html
- Lambrechts, L., Paaijmans, K. P., Fansiri, T., Carrington, L. B., Kramer, L. D., Thomas, M. B., & Scott, T. W. (2011). Impact of daily temperature fluctuations on dengue virus transmission by Aedes aegypti. Proceedings of the National Academy of Sciences of the United States of America, 108(18), 7460–7465. https://doi.org/10. 1073/pnas.1101377108
- Paaijmans, K. P., Blanford, S., Bell, A. S., Blanford, J. I., Read, A. F., & Thomas, M. B. (2010). Influence of climate on malaria transmission depends on daily temperature variation. Proceedings of the National Academy of Sciences of the United States of America, 107(34), 15135–15139. https://doi.org/10.1073/pnas.1006422107
- Kalnay, E., & Cai, M. (2003). Impact of urbanization and land-use change on climate. Nature, 423(6939), 528–531. https://doi.org/10.1038/nature01675
- Thyholt, M., & Hestnes, A. G. (2008). Heat supply to low-energy buildings in district heating areas: Analyses of CO2 emissions and electricity supply security. Energy and Buildings, 40(2), 131–139. https://doi.org/10.1016/ J.ENBUILD.2007.01.016

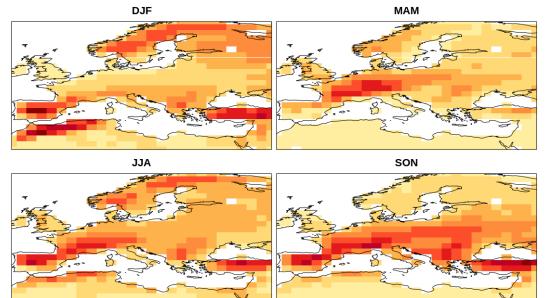
## 15.7.7 Example plots

Mean number of days exceeding the Diurnal Temperature Range (DTR) simulated during the historical period (1961-1990) by 5 degrees during the period 2030-2080. The result is derived from one RCP 8.5 scenario simulated by MPI-ESM-MR.

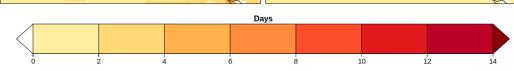
# 15.8 Eady growth rate

#### 15.8.1 Overview

This recipe computes the maximum Eady Growth Rate and performs the annual and seasonal means, storing the results for each dataset. For the seasonal means, the results are plotted over the North-Atlantic region for the selected pressure levels.



Number of days exceeding the DTR by 5 degrees during the period 2030 - 2080



#### 15.8.2 Available recipes and diagnostics

Recipes are stored in esmvaltool/recipes/

• recipe\_eady\_growth\_rate.yml

Diagnostics are stored in esmvaltool/diag\_scripts/eady\_growth\_rate/

• eady\_growth\_rate.py: Computes and stores the eady growth rate. Plots can be produced for the seasonal mean over the North Atlantic region.

#### 15.8.3 User settings in recipe

Script eady\_growth\_rate.py

Required settings for script

• time\_statistic: Set to 'annual' to compute the annual mean. Set to 'seasonal' to compute the seasonal mean.

Optional settings for script

• plot\_levels: list of pressure levels to be plotted for the seasonal mean. If not specified, all levels will be plotted.

#### 15.8.4 Variables

- ta (atmos, monthly mean, longitude latitude level time)
- zg (atmos, monthly mean, longitude latitude level time)
- ua (atmos, monthly mean, longitude latitude level time)

#### 15.8.5 References

- Moreno-Chamarro, E., Caron, L-P., Ortega, P., Loosveldt Tomas, S., and Roberts, M. J., Can we trust CMIP5/6 future projections of European winter precipitation?. Environ. Res. Lett. 16 054063
- Brian J Hoskins and Paul J Valdes. On the existence of storm-tracks. Journal of the atmospheric sciences, 47(15):1854–1864, 1990.

#### 15.8.6 Example plots

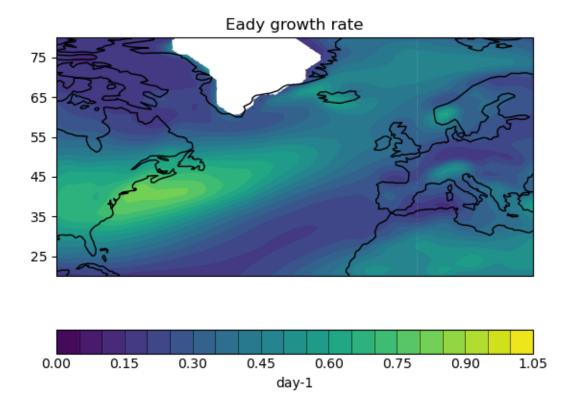


Fig. 21: Eady Growth Rate values over the North-Atlantic region at 70000 Pa.

# 15.9 Extreme Events Indices (ETCCDI)

#### 15.9.1 Overview

This diagnostic uses the standard climdex.pcic.ncdf R library to compute the 27 climate change indices specified by the joint CCI/CLIVAR/JCOMM Expert Team (ET) on Climate Change Detection and Indices http://etccdi.pacificclimate. org/. The needed input fields are daily average precipitation flux and minimum, maximum and average daily surface temperatures. The recipe reproduces panels of figure 9.37 of the IPCC AR5 report, producing both a Gleckler plot, with relative error metrics for the CMIP5 temperature and precipitation extreme indices, and timeseries plots comparing the ensemble spread with observations. For plotting 1 to 4 observational reference datasets are supported. If no observational reference datasets are given, the plotting routines do not work, however, index generation without plotting is still possible. All datasets are regridded to a common grid and considered only over land.

## 15.9.2 Available recipes and diagnostics

Recipes are stored in recipes/

• recipe\_extreme\_events.yml

Diagnostics are stored in diag\_scripts/extreme\_events/

• ExtremeEvents.r

and subroutines

- common\_climdex\_preprocessing\_for\_plots.r
- make\_Glecker\_plot2.r
- make\_timeseries\_plot.r
- cfg\_climdex.r
- cfg\_extreme.r

## 15.9.3 User settings

Required settings for script

- reference\_datasets: list containing the reference datasets to compare with
- timeseries\_idx: list of indices to compute for timeseries plot. The syntax is "XXXETCCDI\_TT", where "TT" can be either "yr" or "mon" (yearly or monthly indices are computed) and "XXX" can be one of the following: "altcdd", "altcsdi", "altcwd", "altwsdi", "cdd", "csdi", "cwd", "dtr", "fd", "gsl", "id", "preptot", "r10mm", "r1mm", "r20mm", "r95p", "r99p", "rx1day", "rx5day", "sdi", "su", "tn10p", "tn90p", "tnn", "tnx", "tr", "tx10p", "tx90p", "txn", "txn", "tx10p", "tx90p", "tx90p", "tx10p", "tx90p", "
- gleckler\_idx: list of indices to compute for Gleckler plot. Same syntax as above. The diagnostic computes all unique indices specified in either gleckler\_idx or timeseries\_idx. If at least one "mon" index is selected, the indices are computed but no plots are produced.
- base\_range: a list of two years to specify the range to be used as "base range" for climdex (the period in which for example reference percentiles are computed)

#### Optional settings for script

• regrid\_dataset: name of dataset to be used as common target for regridding. If missing the first reference dataset is used

- mip\_name: string containing the name of the model ensemble, used for titles and labels in the plots (default: "CMIP")
- analysis\_range: a list of two years to specify the range to be used for the analysis in the plots. The input data will need to cover both analysis\_range and base\_range. If missing the full period covered by the input datasets will be used.
- ts\_plt: (logical) if to produce the timeseries or not (default: true)
- glc\_plt: (logical) if to produce the Gleckler or not (default: true)
- climdex\_parallel: number of parallel threads to be used for climdex calculation (default: 4). Also the logical false can be passed to switch off parallel computation.
- normalize: (logical) if to detrend and normalize with the standard deviation for the datasets for use in the timeseries plot. When this option is used the data for the following indices are detrended and normalized in the timeseries plots: "altcdd", "altcsdi", "altcwd", "altwsdi", "cdd", "cwd", "dtr", "fd", "gsl", "id", "prcptot", "r10mm", "r1mm", "r20mm", "r95p", "r99p", "rx1day", "rx5day", "sdii", "su", "tnn", "tnx", "tr", "txn", "txn", "txx" (default: false)

Additional optional setting controlling the plots:

- Timeseries plots:
  - ts\_png\_width: width for png figures (dafult: 640)
  - ts\_png\_height: height for png figures (default: 480)
  - ts\_png\_units: units for figure size (default: "px")
  - ts\_png\_pointsize: fontsize (default: 12)
  - ts\_png\_bg: background color (default: "white")
  - ts\_col\_list: list of colors for lines (default: ["dodgerblue2", "darkgreen", "firebrick2", "darkorchid", "aquamarine3"]``)
  - ts\_lty\_list: list of linetypes (default: [1, 4, 2, 3, 5])
  - ts\_lwd\_list: list of linewidths (default: [2, 2, 2, 2, 2])
- Gleckler plot:
  - gl\_png\_res: height for png figures (default: 480). The width of the figure is computed automatically.
  - gl\_png\_units: units for figure size (default: "px")
  - gl\_png\_pointsize: fontsize (default: 12)
  - gl\_png\_bg: background color (default: "white")
  - gl\_mar\_par: page margins vector (default: [10, 4, 3, 14])
  - gl\_rmsespacer: spacing of RMSE column (default: 0.01)
  - gl\_scaling\_factor: scaling factor for colorscale height (default: 0.9)
  - gl\_text\_scaling\_factor: scaling factor for text size (default: 1.0)
  - gl\_xscale\_spacer\_rmse: horizontal posizion of coloured colorbar (default: 0.05)
  - gl\_xscale\_spacer\_rmsestd: horizontal posizion of gray colorbar (default: 0.05)
  - gl\_symb\_scaling\_factor: scaling factor for white "symbol" square explaining the partition (default: 1.0)
  - gl\_symb\_xshift: horizontal position of the symbol box (default: 0.2)
  - gl\_symb\_yshift: vertical position of the symbol box (default: 0.275)

- gl\_text\_symb\_scaling\_factor: scaling factor for text to be used for symbol box (default: 0.5)

#### 15.9.4 Variables

- tas (atmos, daily mean, longitude latitude time)
- tasmin (atmos, daily minimum, longitude latitude time)
- tasmax (atmos, daily maximum, longitude latitude time)
- pr (atmos, daily mean, longitude latitude time)

#### 15.9.5 Observations and reformat scripts

None.

#### 15.9.6 References

- Zhang, X., Alexander, L., Hegerl, G. C., Jones, P., Klein Tank, A., Peterson, T. C., Trewin, B., Zwiers, F. W., Indices for monitoring changes in extremes based on daily temperature and precipitation data, WIREs Clim. Change, doi:10.1002/wcc.147, 2011
- Sillmann, J., V. V. Kharin, X. Zhang, and F. W. Zwiers, Climate extreme indices in the CMIP5 multi-model ensemble. Part 1: Model evaluation in the present climate. J. Geophys. Res., doi:10.1029/2012JD018390, 2013

#### 15.9.7 Example plots

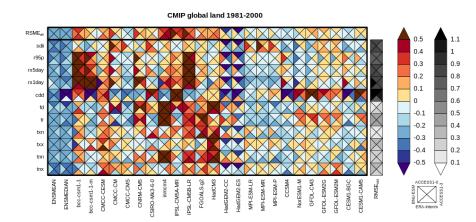


Fig. 22: Portrait plot of relative error metrics for the CMIP5 temperature and precipitation extreme indices evaluated over 1981-2000. Reproduces Fig. 9.37 of the IPCC AR5 report, Chapter 9.

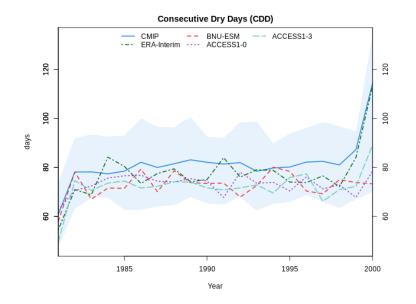


Fig. 23: Timeseries of the Consecutive Dry Days index over 1981-2000 for a selection of CMIP5 models, the CMIP5 multi-model mean (CMIP) and ERA-Interim. Shading is used to reproduce the multi-model spread.

## **15.10 Combined Climate Extreme Index**

#### 15.10.1 Overview

The goal of this diagnostic is to compute time series of a number of extreme events: heatwave, coldwave, heavy precipitation, drought and high wind. Then, the user can combine these different components (with or without weights). The result is an index similar to the Climate Extremes Index (CEI; Karl et al., 1996), the modified CEI (mCEI; Gleason et al., 2008) or the Actuaries Climate Index (ACI; American Academy of Actuaries, 2018). The output consists of a netcdf file containing the area-weighted and multi-model multi-metric index. This recipe expects data of daily temporal resolution, and the running average is computed based on the user-defined window length (e.g. a window length of 5 would compute the 5-day running mean).

In recipe\_extreme\_index.yml, after defining the area and reference and projection period, the weigths for each metric selected. The options are

- weight\_t90p the weight of the number of days when the maximum temperature exceeds the 90th percentile,
- weight\_t10p the weight of the number of days when the minimum temperature falls below the 10th percentile,
- weight\_Wx the weight of the number of days when wind power (third power of wind speed) exceeds the 90th percentile,
- weight\_cdd the weight of the maximum length of a dry spell, defined as the maximum number of consecutive days when the daily precipitation is lower than 1 mm, and
- weight\_rx5day the weight of the maximum precipitation accumulated during 5 consecutive days.

#### 15.10.2 Available recipes and diagnostics

Recipes are stored in recipes/

recipe\_extreme\_index.yml

Diagnostics are stored in diag\_scripts/magic\_bsc/

• extreme\_index.R

#### 15.10.3 User settings

User setting files are stored in recipes/

1. recipe\_extreme\_index.yml

Required settings for script

- weight\_t90p: 0.2 (from 0 to 1, the total sum of the weight should be 1)
- weight\_t10p: 0.2 (from 0 to 1, the total sum of the weight should be 1)
- weight\_Wx: 0.2 (from 0 to 1, the total sum of the weight should be 1)
- weight\_rx5day: 0.2 (from 0 to 1, the total sum of the weight should be 1)
- weight\_cdd: 0.2 (from 0 to 1, the total sum of the weight should be 1)
- running\_mean: 5 (depends on the length of the future projection period selected, but recommended not greater than 11)

#### 15.10.4 Variables

- tasmax (atmos, daily, longitude, latitude, time)
- tasmin (atmos, daily, longitude, latitude, time)
- sfcWind (atmos, daily, longitude, latitude, time)
- pr (atmos, daily, longitude, latitude, time)

## 15.10.5 Observations and reformat scripts

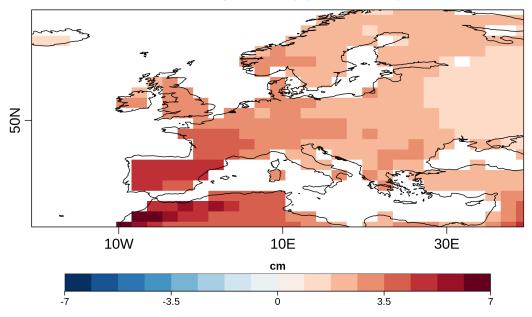
None

#### 15.10.6 References

- Alexander L.V. and Coauthors (2006). Global observed changes in daily climate extremes of temperature and precipitation. J. Geophys. Res., 111, D05109. https://doi.org/10.1029/2005JD006290
- American Academy of Actuaries, Canadian Institute of Actuaries, Casualty Actuarial Society and Society of Actuaries. Actuaries Climate Index. http://actuariesclimateindex.org (2018-10-06).
- Donat, M., and Coauthors (2013). Updated analyses of temperature and precipitation extreme indices since the beginning of the twentieth century: The HadEX2 dataset. J. Geophys. Res., 118, 2098–2118, https://doi.org/10. 1002/jgrd.50150.

- Fouillet, A., Rey, G., Laurent, F., Pavillon, G. Bellec, S., Guihenneuc-Jouyaux, C., Clavel J., Jougla, E. and Hémon, D. (2006) Excess mortality related to the August 2003 heat wave in France. Int. Arch. Occup. Environ. Health, 80, 16–24. https://doi.org/10.1007/s00420-006-0089-4
- Gleason, K.L., J.H. Lawrimore, D.H. Levinson, T.R. Karl, and D.J. Karoly (2008). A Revised U.S. Climate Extremes Index. J. Climate, 21, 2124-2137 https://doi.org/10.1175/2007JCLI1883.1
- Meehl, G. A., and Coauthors (2000). An introduction to trends inextreme weather and climate events: Observations, socio-economic impacts, terrestrial ecological impacts, and model projections. Bull. Amer. Meteor. Soc., 81, 413–416. doi: 10.1175/1520-0477(2000)081<0413:AITTIE>2.3.CO;2
- Whitman, S., G. Good, E. R. Donoghue, N. Benbow, W. Y. Shou and S. X. Mou (1997). Mortality in Chicago attributed to the July 1995 heat wave. Amer. J. Public Health, 87, 1515–1518. https://doi.org/10.2105/AJPH. 87.9.1515
- Zhang, Y., M. Nitschke, and P. Bi (2013). Risk factors for direct heat-related hospitalization during the 2009 Adelaide heat-wave: A case crossover study. Sci. Total Environ., 442, 1–5. https://doi.org/10.1016/j.scitotenv. 2012.10.042
- Zhang, X., Alexander, L., Hegerl, G. C., Jones, P., Tank, A. K., Peterson, T. C., Trewin, B. and Zwiers, F. W. (2011). Indices for monitoring changes in extremes based on daily temperature and precipitation data. WIREs Clim Change, 2: 851-870. doi:10.1002/wcc.147. https://doi.org/10.1002/wcc.147

## 15.10.7 Example plots



#### Index for t90p 2020-2040 (rcp85 MPI-ESM-MR)

Average change in the heat component (t90p metric) of the Combined Climate Extreme Index for the 2020-2040 compared to the 1971-2000 reference period for the RCP 8.5 scenario simulated by MPI-ESM-MR.

# 15.11 Diagnostics of stratospheric dynamics and chemistry

#### 15.11.1 Overview

This recipe reproduces the figures of Eyring et al. (2006) The following plots are reproduced:

- Vertical profile climatological mean bias of climatological mean for selected seasons and latitudinal region.
- Vertical and latitudinal profile of climatological mean for selected seasons this figure and setting is valid for figure 5 (CH4) figure 6 (H2O) figure 11 (HCL) figure 13 (tro3).
- Total ozone anomalies at different latitudinal band and seasons.

#### 15.11.2 Available recipes and diagnostics

Recipes are stored in esmvaltool/recipes/

• recipe\_eyring06jgr.yml

Diagnostics are stored in esmvaltool/diag\_scripts/eyring06jgr/

- eyring06jgr\_fig01.ncl
- eyring06jgr\_fig05a.ncl
- eyring06jgr\_fig05b.ncl
- eyring06jgr\_fig15.ncl

#### 15.11.3 User settings in recipe

- 1. Preprocessor
  - regrid\_interp\_lev\_zonal: Regridding and interpolation reference\_dataset levels used by eyring06jgr\_fig01 and eyring06jgr\_fig05
  - zonal : Regridding and zonal mean used by eyring06jgr\_fig15
- 2. Script <eyring06jgr\_fig01.ncl>

Required settings for script

- latmin: array of float, min lat where variable is averaged, i.e. [60., 60., -90., -90.]
- latmax: array of float, and max lat where variable is averaged, i.e. [90., 90., -60., -60.]
- season: array of string., season when variable is averaged, i.e. ["DJF", "MAM", "JJA", "SON"]
- XMin: array of float, min limit X axis [-30., -30., -30., -30.]
- XMax: array of float, max limit X axis [20., 20., 20., 20.]
- levmin: array of float, min limit Y axis [1., 1., 1., 1.]
- levmax: array of float, max limit Y axis [350., 350., 350., 350.]

Optional settings for script

- start\_year: int, year when start the climatology calculation [1980] (default max among the models start year).
- end\_year:int, year when end the climatology calculation [1999] (default min among the models end year).

• multimean: bool, calculate multi-model mean, (i.e. False/True) (default False).

Required settings for variables

- preprocessor: regrid\_interp\_lev.
- reference\_dataset: name of the reference model or observation for regridding and bias calculation (e.g. ERA-Interim").
- mip: Amon.

#### 15.11.4 Variables

• ta (atmos, monthly mean, longitude latitude level time)

#### 15.11.5 Example plots

## 15.12 Ozone and associated climate impacts

#### 15.12.1 Overview

This recipe is implemented into the ESMValTool to evaluate atmospheric chemistry and the climate impact of stratospheric ozone changes. It reproduces selected plots from Eyring et al. (2013).

The following plots are reproduced:

· Zonal mean of long-term zonal wind with linear trend

#### 15.12.2 Available recipes and diagnostics

Recipes are stored in esmvaltool/recipes/

• recipe\_eyring13jgr\_12.yml

Diagnostics are stored in esmvaltool/diag\_scripts/eyring13jgr/

eyring13jgr\_fig12.ncl

#### 15.12.3 User settings in recipe

- 1. Preprocessor
  - zonal : Regridding and zonal mean used by eyring13jgr\_fig12
- 2. Script <eyring13jgr\_fig12.ncl>

Required settings for script

• e13fig12\_exp\_MMM: name of the experiments for the MMM

Optional settings for script

- e13fig12\_start\_year: year when to start the climatology calculation
- e13fig12\_end\_year: year when to end the climatology calculation
- e13fig12\_multimean: calculate multimodel mean (default: False)

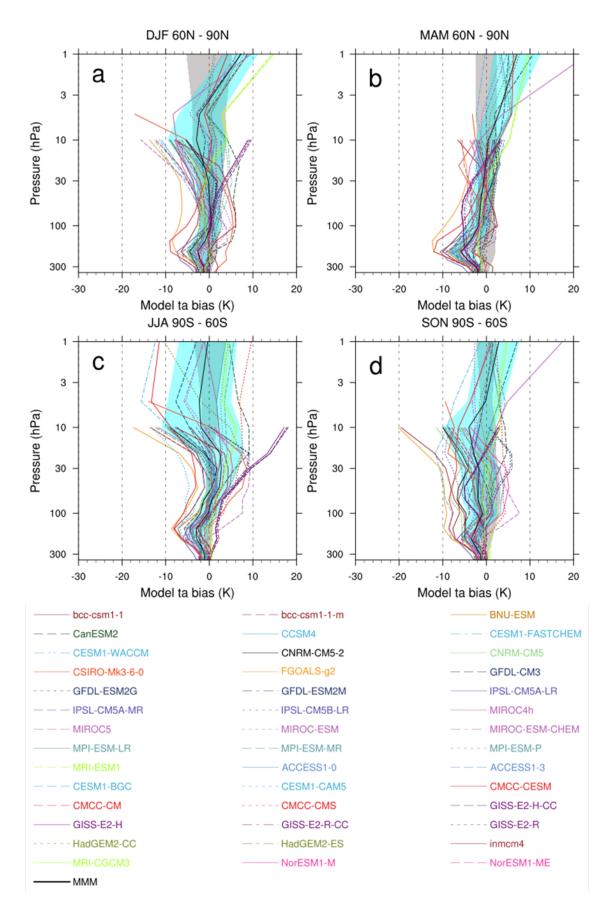


Fig. 24: Climatological mean temperature biases for (top) 60–90N and (bottom) 60–90S for the (left) winter and (15 ght) spring seasons. The climatological mean sport the CCMs and ERA-Interim data from 1980 to 1999 are included. Biases are calculated relative to ERA-Interim reanalyses. The grey area shows ERA-Interim plus and minus 1 standard deviation (s) about the climatological mean. The turquoise area shows plus and minus 1 standard deviation about the multi-model mean.

• e13fig12\_season: season (default: ANN (annual))

Required settings for variables

- preprocessor: zonal
- reference\_dataset: name of the reference model or observation for regridding and bias calculation (e.g. ERA5).
- mip: Amon.

#### 15.12.4 Variables

• ua (atmos, monthly mean, longitude latitude level time)

#### 15.12.5 Observations and reformat scripts

• ERA5 Reformatting with: recipes/cmorizers/recipe\_era5.yml

#### 15.12.6 Example plots

# 15.13 Spatially resolved evaluation of ESMs with satellite columnaveraged CO<sub>2</sub>

#### 15.13.1 Overview

This recipe reproduces the figures of Gier et al. (2020). It uses satellite column-averaged  $CO_2$  data to evaluate ESMs by plotting several quantities such as timeseries, seasonal cycle and growth rate in different areas.

#### 15.13.2 Available recipes and diagnostics

Recipes are stored in esmvaltool/recipes/

• recipe\_gier20bg.yml

Diagnostics are stored in diag\_scripts/

Diagnostics are stored in esmvaltool/diag\_scripts/xco2\_analysis/

- carbon\_plots.ncl: plot script for panel plots
- delta\_T.ncl: IAV of growth rate against growing season temperature Figure C1
- global\_maps.ncl: global maps for seasonal cycle amplitude Figures 5, 6
- main.ncl: Timeseries and histogram Figures 3, 4
- panel\_plots.ncl: scatter plot of SCA/GR vs variable Figures 7, 9, B1, B2
- sat\_masks.ncl: data coverage of input data Figures 1, 8
- stat.ncl: auxiliary functions for GR, SCA computation
- station\_comparison.ncl: comparison of surface and column data Figure 2

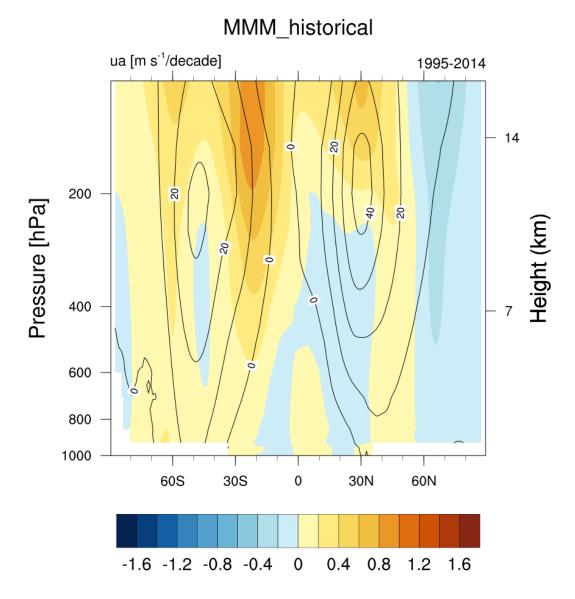


Fig. 25: Long-term mean (thin black contour) and linear trend (colour) of zonal mean DJF zonal winds for the multimodel mean CMIP6 over 1995-2014

#### 15.13.3 User settings in recipe

- 1. Preprocessor
  - conv\_units: converts units to plot-units
  - mmm\_ref: calculates multi-model mean and regrids to ref dataset
  - mmm\_2x2: computes multi-model mean on 2x2 grid
  - mmm: computes multi-model mean for 3D variable, 5x5 grid with specific pressure levels
- 2. Script xco2\_analysis/delta\_T.ncl
  - Required diag\_script\_info attributes:
    - region: region to average over
    - masking: the kind of masking to apply prior to region average (possible options: obs, land, sciamachy, gosat, none)
    - var\_order: First main variable, then temperature variable to compare

#### • Optional diag\_script\_info attributes:

- styleset: styleset for color coding panels
- output\_file\_type: output file type for plots, default: config\_user -> png
- var\_plotname: NCL string formatting how variable should be named in plots defaults to short\_name if not assigned.
- 3. Script xco2\_analysis/global\_maps.ncl:
  - Required diag\_script\_info attributes:
    - contour\_max\_level: maximum value displayed for seasonal cycle amplitude contour plot
  - Optional diag\_script\_info attributes:
    - output\_file\_type: output file type for plots, default: config\_user -> png
- 4. Script xco2\_analysis/main.ncl:
  - Required diag\_script\_info attributes:
    - styleset: styleset to use for plotting colors, linestyles...
    - region: latitude range for averaging
    - masking: different masking options are available to use on dataset: (possible options: none, obs)
    - ensemble\_mean: if true calculates multi-model mean only accounting for the ensemble member named in "ensemble\_refs"

#### • Optional diag\_script\_info attributes:

- output\_file\_type: output file type for plots, default: config\_user -> png
- ensemble\_refs: list of model-ensemble pairs to denote which ensemble member to use for calculating multi-model mean. required if ensemble\_mean = true
- var\_plotname: String formatting how variable should be named in plots defaults to short\_name if not assigned
- 5. Script xco2\_analysis/panel\_plots.ncl:
  - Required diag\_script\_info attributes:

- styleset: styleset to use for plotting colors, linestyles...
- region: latitude range for averaging
- masking: different masking options are available to use on dataset: (possible options: obs, land, sciamachy, gosat, none)
- obs\_in\_panel: True if observations should be included in plot
- area\_avg: Type of area averaging: "full-area" normal area-average "lat-first" calculate zonal means first, then average these
- plot\_var2\_mean: If True adds mean of seasonal cycle to panel as string.

#### Optional diag\_script\_info attributes:

- output\_file\_type: output file type for plots, default: config\_user -> png
- var\_plotname: String formatting how variable should be named in plots defaults to short\_name if not assigned
- 6. Script xco2\_analysis/sat\_masks.ncl:

#### • Optional diag\_script\_info attributes:

- output\_file\_type: output file type for plots, default: config\_user -> png
- var\_plotname: String formatting how variable should be named in plots defaults to short\_name if not assigned
- c3s\_plots: Missing value plots seperated by timeseries of c3s satellites
- 7. Script xco2\_analysis/station\_comparison.ncl:
  - Required diag\_script\_info attributes:
    - var\_order: in this case xco2, co2, co2s column averaged with obs dataset first, then 2D variable, followed by surface stations
  - Optional diag\_script\_info attributes:
    - output\_file\_type: output file type for plots, default: config\_user -> png
    - var\_plotnames: String formatting how variables should be named in plots defaults to short\_name if not assigned
    - overwrite\_altitudes: Give other altitude values than the ones attached in the station data.
       Valid if altitude changes and timeseries spans range with different sample altitude. Caveat: If used, need to give altitude values for all stations.
    - output\_map: boolean if stations to be displayed on map. As this requires finetuning, currently
      only implemented for station set of (ASK, CGO, HUN, LEF, WIS) following the paper. Change
      for different plot inset locations, if others are desired.

#### 15.13.4 Variables

- *xco2* (atmos, monthly, longitude, latitude, time)
- *co2s* (atmos, monthly, longitude, latitude, time)
- co2 (atmos, monthly, pressure, longitude, latitude, time)
- *tas* (atmos, monthly, longitude, latitude, time)
- tasa (atmos, monthly, longitude, latitude, time)

#### 15.13.5 Observations and reformat scripts

- CDS-XCO2 (*xco2*)
- ESRL (*co2s*)
- GISTEMP (tasa)
- MODIS (land cover map, auxiliary data folder)

#### 15.13.6 References

• Gier, B. K., Buchwitz, M., Reuter, M., Cox, P. M., Friedlingstein, P., and Eyring, V.: Spatially resolved evaluation of Earth system models with satellite column-averaged CO2, Biogeosciences, 17, 6115–6144, https://doi.org/10. 5194/bg-17-6115-2020, 2020.

#### 15.13.7 Example plots

## 15.14 Heat wave and cold wave duration

#### 15.14.1 Overview

The goal of this diagnostic is to estimate the relative change in heat/cold wave characteristics in future climates compared to a reference period using daily maximum or minimum temperatures.

The user can select whether to compute the frequency of exceedances or non-exceedances, which corresponds to extreme high or extreme low temperature events, respectively. The user can also select the minimum duration for an event to be classified as a heat/cold wave and the season of interest.

The diagnostic calculates the number of days in which the temperature exceeds or does not exceeds the necessary threshold for a consecutive number of days in future climate projections. The result is an annual time series of the total number of heat/cold wave days for the selected season at each grid point. The final output is the average number of heat/cold wave days for the selected season in the future climate projections.

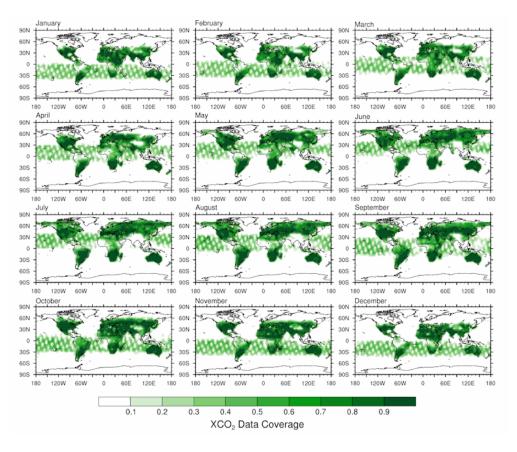


Fig. 26: Mean fractional coverage of monthly satellite data.

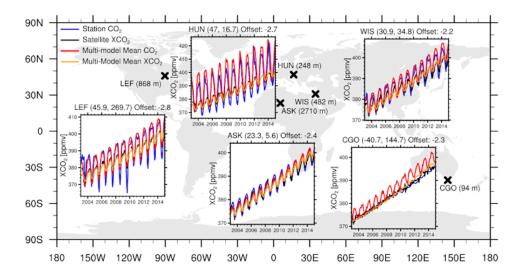


Fig. 27: Comparison of time series from satellite, in situ, and models sampled accordingly. Caveat: inset plot positions are hardcoded.

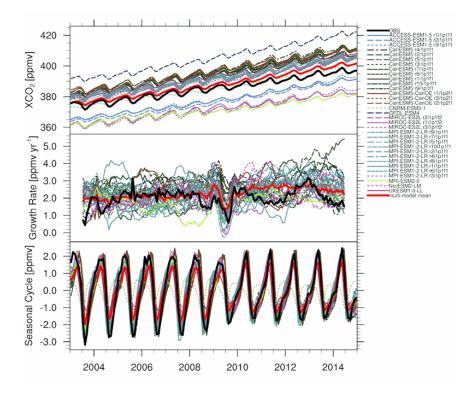


Fig. 28: Timeseries with panels depicting growth rate and seasonal cycle.

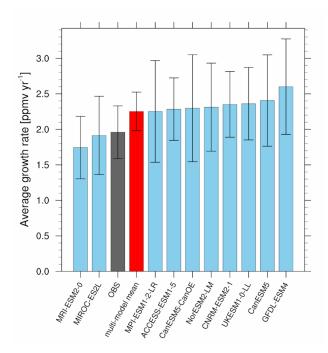


Fig. 29: Barplot of the growth rate, averaged over all years, with standard deviation of interannual variability.

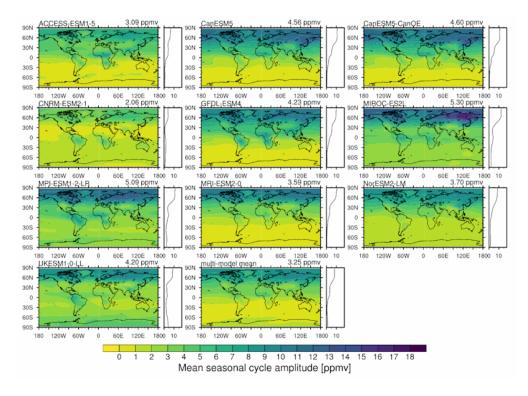


Fig. 30: Panel plot of spatially resolved seasonal cycle amplitude for all models, including a zonal average sidepanel.

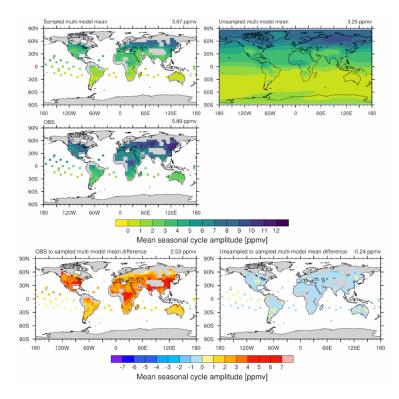


Fig. 31: Seasonal cycle amplitude map comparing influence of sampling, and difference to observations.

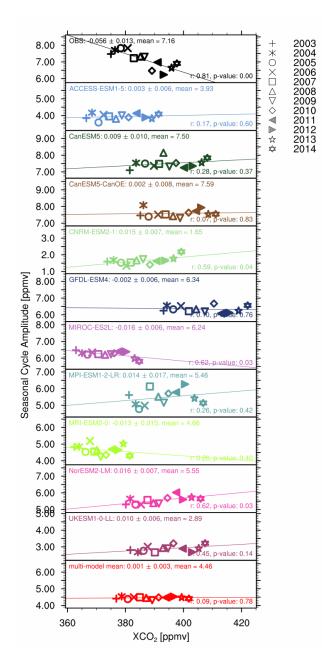


Fig. 32: Panel plots showing seasonal cycle amplitude against XCO<sub>2</sub>, includes regression line and p-value.

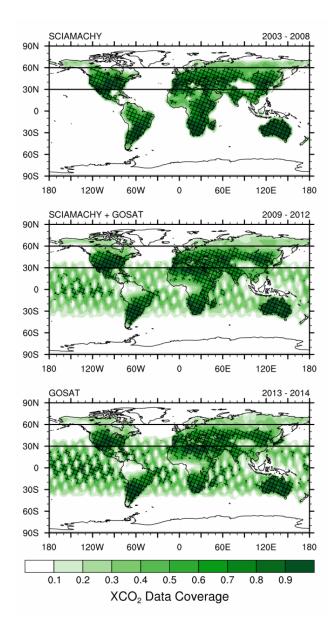


Fig. 33: Mean spatial data coverage for different satellites.

#### 15.14.2 Available recipes and diagnostics

Recipes are stored in recipes/

recipe\_heatwaves\_coldwaves.yml

Diagnostics are stored in diag\_scripts/magic\_bsc/

• extreme\_spells.R: calculates the heatwave or coldwave duration.

## 15.14.3 User settings

User setting files are stored in recipes/

1. recipe\_heatwaves\_coldwaves.yml

Required settings for script

- quantile: quantile defining the exceedance/non-exceedance threshold
- min\_duration: Min duration in days of a heatwave/coldwave event
- Operator: either '>' for exceedances or '<' for non-exceedances
- season: 'summer' or 'winter

## 15.14.4 Variables

• tasmax or tasmin (atmos, daily, longitude, latitude, time)

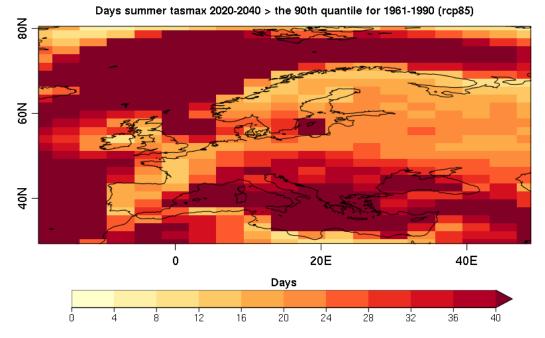
## 15.14.5 Observations and reformat scripts

None

## 15.14.6 References

- Cardoso, S., Marta-Almeida, M., Carvalho, A.C., & Rocha, A. (2017). Heat wave and cold spell changes in Iberia for a future climate scenario. International Journal of Climatology, 37(15), 5192-5205. https://doi.org/ 10.1002/joc.5158
- Ouzeau, G., Soubeyroux, J.-M., Schneider, M., Vautard, R., & Planton, S. (2016). Heat waves analysis over France in present and future climate: Application of a new method on the EURO-CORDEX ensemble. Climate Services, 4, 1-12. https://doi.org/10.1016/J.CLISER.2016.09.002
- Wang, Y., Shi, L., Zanobetti, A., & Schwartz, J. D. (2016). Estimating and projecting the effect of cold waves on mortality in 209 US cities. Environment International, 94, 141-149. https://doi.org/10.1016/j.envint.2016. 05.008
- Zhang, X., Hegerl, G., Zwiers, F. W., & Kenyon, J. (2005). Avoiding inhomogeneity in percentile-based indices of temperature extremes. Journal of Climate, 18(11), 1641-1651. https://doi.org/10.1175/JCLI3366.1

#### 15.14.7 Example plots



Mean number of summer days during the period 2060-2080 when the daily maximum near-surface air temperature exceeds the 80th quantile of the 1971-2000 reference period. The results are based on one RCP 8.5 scenario simulated by BCC-CSM1-1.

# 15.15 Hydroclimatic intensity and extremes (HyInt)

#### 15.15.1 Overview

The HyInt tool calculates a suite of hydroclimatic and climate extremes indices to perform a multi-index evaluation of climate models. The tool firstly computes a set of 6 indices that allow to evaluate the response of the hydrological cycle to global warming with a joint view of both wet and dry extremes. The indices were selected following Giorgi et al. (2014) and include the simple precipitation intensity index (SDII) and extreme precipitation index (R95), the maximum dry spell length (DSL) and wet spell length (WSL), the hydroclimatic intensity index (HY-INT), which is a measure of the overall behaviour of the hydroclimatic cycle (Giorgi et al., 2011), and the precipitation area (PA), i.e. the area over which at any given day precipitation occurs, (Giorgi et al., 2014). Secondly, a selection of the 27 temperature and precipitation -based indices of extremes from the Expert Team on Climate Change Detection and Indices (ETCCDI) produced by the climdex (https://www.climdex.org) library can be ingested to produce a multi-index analysis. The tool allows then to perform a subsequent analysis of the selected indices calculating timeseries and trends over predefined continental areas, normalized to a reference period. Trends are calculated using the R *lm* function and significance testing performed with a Student T test on non-null coefficients hypothesis. Trend coefficients are stored together with their statistics which include standard error, t value and Pr(>|t|). The tool can then produce a variety of types of plots including global and regional maps, maps of comparison between models and a reference dataset, timeseries with their spread, trend lines and summary plots of trend coefficients.

The hydroclimatic indices calculated by the recipe\_hyint.yml and included in the output are defined as follows:

- PRY = mean annual precipitation
- INT = mean annual precipitation intensity (intensity during wet days, or simple precipitation intensity index SDII)

- WSL = mean annual wet spell length (number of consecutive days during each wet spell)
- DSL = mean annual dry spell lenght (number of consecutive days during each dry spell)
- PA = precipitation area (area over which of any given day precipitation occurs)
- R95 = heavy precipitation index (percent of total precipitation above the 95% percentile of the reference distribution)
- HY-INT = hydroclimatic intensity. HY-INT = normalized(INT) x normalized(DSL).

The recipe\_hyint\_extreme\_events.yml includes an additional call to the *Extreme Events Indices (ETCCDI)* diagnostics, which allows to calculate the ETCCDI indices and include them in the subsequent analysis together with the hydroclimatic indices. All of the selected indices are then stored in output files and figures.

## 15.15.2 Available recipes and diagnostics

Recipes are stored in recipes/

- recipe\_hyint.yml (evaluating the 6 hydroclimatic indices, performing trend analysis and plotting)
- recipe\_hyint\_extreme\_events.yml (similar to the recipe\_hyint.yml but with an additional call to the *Extreme Events Indices* (*ETCCDI*) diagnostic for calculation of ETCCDI indices and inclusion of them in the trend analysis and plotting)

Diagnostics are stored in diag\_scripts/hyint/

• hyint.R

and subroutines

- hyint\_diagnostic.R
- hyint\_functions.R
- hyint\_parameters.R
- hyint\_plot\_trends.R
- hyint\_etccdi\_preproc.R
- hyint\_metadata.R
- hyint\_plot\_maps.R
- hyint\_preproc.R
- hyint\_trends.R

See details of the extreme\_events diagnostics under recipe\_extreme\_events.yml.

## 15.15.3 Known issues

#### recipe\_hyint\_extreme\_events.yml

Call to the *Extreme Events Indices (ETCCDI)* diagnostic requires the ncdf4.helpers library, which is currently unavailable on CRAN. Users need therefore to install the library manually, e.g. through the following commands to download the package tarball from CRAN archive, install it and remove the package tarball:

- url <- "https://cran.r-project.org/src/contrib/Archive/ncdf4.helpers/ncdf4.helpers\_0.3-3.tar.gz"
- pkgFile <- "ncdf4.helpers\_0.3-3.tar.gz"
- download.file(url = url, destfile = pkgFile)

- install.packages(pkgs=pkgFile, type="source", repos=NULL)
- unlink(pkgFile)

#### 15.15.4 User settings

#### Required settings for script

- norm\_years: first and last year of reference normalization period to be used for normalized indices
- select\_indices: indices to be analysed and plotted. Select one or more fields from the following list (ordersensitive): "pa\_norm", "hyint", "int\_norm", "r95\_norm", "wsl\_norm", "dsl\_norm", "int", "dsl", "wsl"
- select\_regions: Select regions for timeseries and maps from the following list: GL=Globe, GL60=Global 60S/60N, TR=Tropics (30S/30N), SA=South America, AF=Africa, NA=North America, IN=India, EU=Europe, EA=East-Asia, AU=Australia
- plot\_type: type of figures to be plotted. Select one or more from: 1=lon/lat maps per individual field/exp/multiyear mean, 2=lon/lat maps per individual field exp-ref-diff/multi-year mean, 3=lon/lat maps multi-field/expref-diff/multi-year mean, 11=timeseries over required individual region/exp, 12=timeseries over multiple regions/exp, 13=timeseries with multiple models, 14=summary trend coefficients multiple regions, 15=summary trend coefficients multiple models

Additional settings for recipe\_hyint\_extreme\_events.yml

- call to the extreme\_events diagnostics: see details in recipe\_extreme\_events.yml. Make sure that the base\_range for extreme\_events coincides with the norm\_range of hyint and that all ETCCDI indices that are required to be imported in hyint are calculated by the extreme\_events diagnostics.
- etccdi\_preproc: set to true to pre-process and include ETCCDI indices in hyint
- etccdi\_list\_import: specify the list of ETCCDI indices to be imported, e.g.: "tn10pETCCDI", "tn90pETCCDI", "tx10pETCCDI", "tx90pETCCDI"
- select\_indices: this required settings should here be revised to include the imported indices, e.g.: "pa\_norm", "hyint", "tn10pETCCDI", "tn90pETCCDI", "tx10pETCCDI", "tx90pETCCDI"

#### Optional settings for script (with default setting)

- 1. Data
  - rgrid (false): Define whether model data should be regridded. (a) false to keep original resolution; (b) set desired regridding resolution in cdo format e.g., "r320x160"; (c) "REF" to use resolution of reference model
- 2. Plotting
  - npancol (2): number of columns in timeseries/trends multipanel figures
  - npanrow (3): number of rows in timeseries/trends multipanel figures
  - autolevels (true): select automated (true) or pre-set (false) range of values in plots
  - autolevels\_scale (1): factor multiplying automated range for maps and timeseries
  - autolevels\_scale\_t (1.5): factor multiplying automated range for trend coefficients
- 3. Maps
  - oplot\_grid (false): plot grid points over maps
  - boxregion (false): !=0 plot region boxes over global maps with thickness = abs(boxregion); white (>0) or grey (<0).

- removedesert (false) remove (flag as NA) grid points with mean annual pr < 0.5 mm/day (deserts, Giorgi2014). This affects timeseries and trends calculations too.
- 4. Timeseries and trends
  - weight\_tseries (true): adopt area weights in timeseries
  - trend\_years (false): (a) false = apply trend to all years in dataset; (b) [year1, year2] to apply trend calculation and plotting only to a limited time interval
  - add\_trend (true): add linear trend to plot
  - add\_trend\_sd (false): add dashed lines of stdev range to timeseries
  - add\_trend\_sd\_shade (false): add shade of stdev range to timeseries
  - add\_tseries\_lines (true): plot lines connecting timeseries points
  - add\_zeroline (true): plot a dashed line at y=0
  - trend\_years\_only (false): limit timeseries plotting to the time interval adopted for trend calculation (excluding the normalization period)
  - scale100years (true): plot trends scaled as 1/100 years
  - scalepercent (false): plot trends as percent change

#### 15.15.5 Variables

• pr (atmos, daily mean, longitude latitude time)

Additional variables for recipe\_hyint\_extreme\_events.yml

- tas (atmos, daily mean, longitude latitude time)
- tasmin (atmos, daily mean, longitude latitude time)
- tasmax (atmos, daily mean, longitude latitude time)

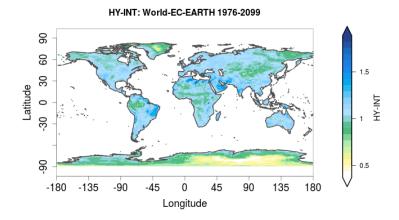
#### 15.15.6 Observations and reformat scripts

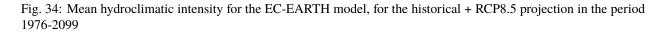
None.

#### 15.15.7 References

- Giorgi et al., 2014, J. Geophys. Res. Atmos., 119, 11,695-11,708, doi:10.1002/2014JD022238
- Giorgi et al., 2011, J. Climate 24, 5309-5324, doi:10.1175/2011JCLI3979.1

#### 15.15.8 Example plots





## 15.16 Implied heat transport from Top of Atmosphere fluxes

#### 15.16.1 Overview

This recipe calculates the implied horizontal heat transport (IHT) due to the spatial anomalies of radiative fluxes at the top of the atmosphere (TOA). The regional patterns of implied heat transport for different components of the TOA fluxes are calculated by solving the Poisson equation with the flux components as source terms. It reproduces the plots in Pearce and Bodas-Salcedo (2023) when the input data is CERES EBAF.

#### 15.16.2 Available recipes and diagnostics

Recipes are stored in esmvaltool/recipes/

- recipe\_iht\_toa.yml calculates the IHT maps for the following radiative fluxes:
  - Total net, SW net, LW net (Figure 2).
  - Total CRE, SW CRE, LW CRE (Figure 4).
  - All-sky and clear-sky reflected SW (Figure 5).
  - The meridional heat transports (MHT) of the fluxes above (Figures 1 and 3).

Diagnostics are stored in esmvaltool/diag\_scripts/iht\_toa/

- single\_model\_diagnostics.py: driver script that produces the plots.
- poisson\_solver.py: solver that calculates the IHTs.

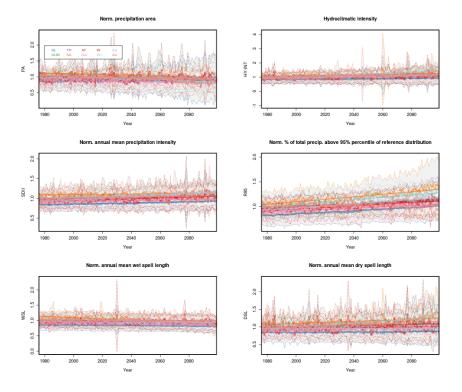


Fig. 35: Timeseries for multiple indices and regions for the ACCESS1-0 model, for the historical + RCP8.5 projection in the period 1976-2099, normalized to the 1976-2005 historical period.

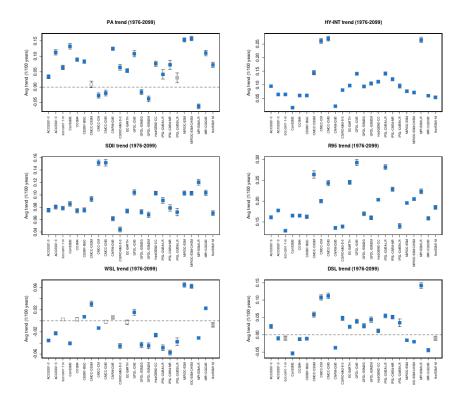


Fig. 36: Multi-model trend coefficients over selected indices for CMIP5 models in the RCP8.5 2006-2099 projection, normalized to the 1976-2005 historical period.

#### 15.16.3 User settings in recipe

There are no user settings in this recipe.

#### 15.16.4 Variables

- rlut (atmos, monthly, longitude latitude time)
- rlutcs (atmos, monthly, longitude latitude time)
- rsutcs (atmos, monthly, longitude latitude time)
- rsut (atmos, monthly, longitude latitude time)
- rsdt (atmos, monthly, longitude latitude time)

#### 15.16.5 Observations and reformat scripts

• CERES-EBAF

#### 15.16.6 References

• Pearce, F. A., and A. Bodas-Salcedo, 2023: Implied Heat Transport from CERES Data: Direct Radiative Effect of Clouds on Regional Patterns and Hemispheric Symmetry. J. Climate, 36, 4019–4030, doi: 10.1175/JCLI-D-22-0149.1.

## 15.16.7 Example plots

## 15.17 Quick insights for climate impact researchers

#### 15.17.1 Overview

Many impact researchers do not have the time and finances to use a large ensemble of climate model runs for their impact analysis. To get an idea of the range of impacts of climate change it also suffices to use a small number of climate model runs. In case a system is only sensitive to annual temperature, one can select a run with a high change and one with a low change of annual temperature, preferably both with a low bias.

This recipe calculates the bias with respect to observations, and the change with respect to a reference period, for a wide range of (CMIP) models. These metrics are tabulated and also visualized in a diagram.

## 15.17.2 Available recipes and diagnostics

Recipes are stored in esmvaltool/recipes/

• recipe\_impact.yml

Diagnostics are stored in esmvaltool/diag\_scripts/

• impact/bias\_and\_change.py: tabulate and visualize bias and change.

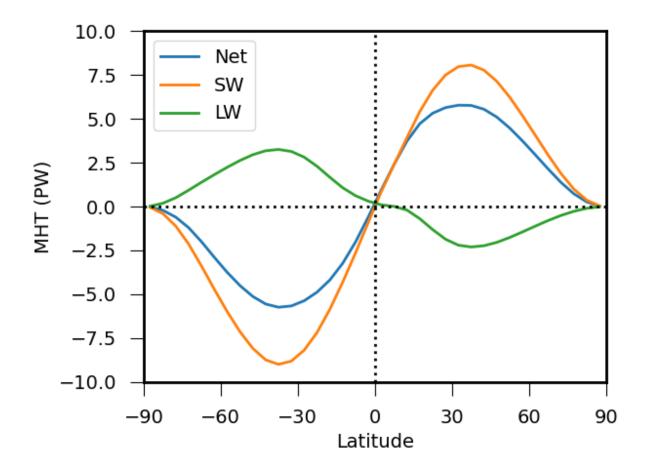


Fig. 37: The implied heat transport due to the total net flux (blue), split into the contributions from the SW (orange) and LW (green).

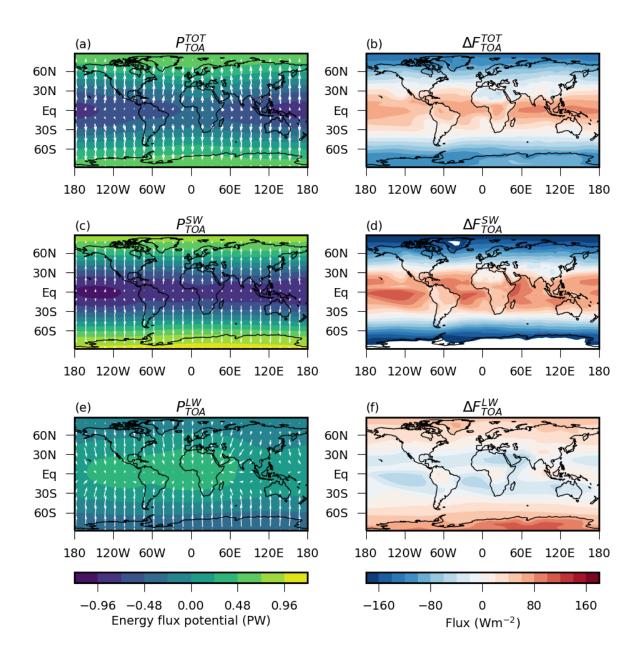


Fig. 38: The energy flux potentials for (a) TOT, (c) SW, and (e) LW fluxes, alongside maps of the spatial anomalies of the fluxes [(b),(d),(f) flux minus global average flux, respectively]. The implied heat transport is calculated as the gradient of the energy flux potential, shown by the white vector arrows for a subset of points to give the overall transport pattern. Heat is directed from the blue minima of the potential field to yellow maxima, with the magnitude implied by the density of contours. All maps of the same type share the same color bar at the bottom of the column.

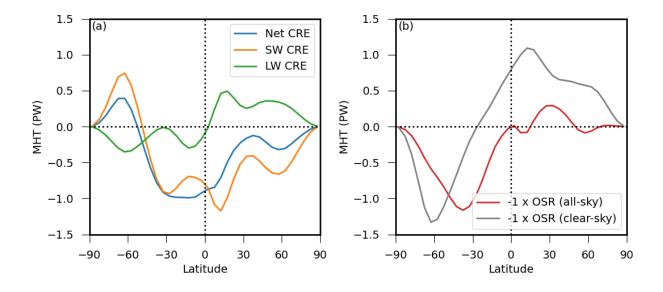


Fig. 39: Direct radiative effects of clouds on the meridional heat transport. (a) Contributions from TOT CRE (blue), SW CRE (orange), and LW CRE (green) fluxes. (b) Contributions from all-sky and clear-sky OSR. In (b), both curves have been multiplied by 1 such that positive heat transport is northward.

#### 15.17.3 User settings in recipe

Script impact.py

Required settings for variables

• tag: 'model' or 'observations', so the diagnostic script knows which datasets to use for the bias calculation. This must be specified for each dataset.

Optional settings for preprocessor

• Region and time settings (both for the future and reference period) can be changed at will.

#### 15.17.4 Variables

- tas (atmos, mon, longitude latitude time)
- pr (atmos, mon, longitude latitude time)
- · any other variables of interest

## 15.17.5 Observations and reformat scripts

• ERA5 data can be used via the native6 project.

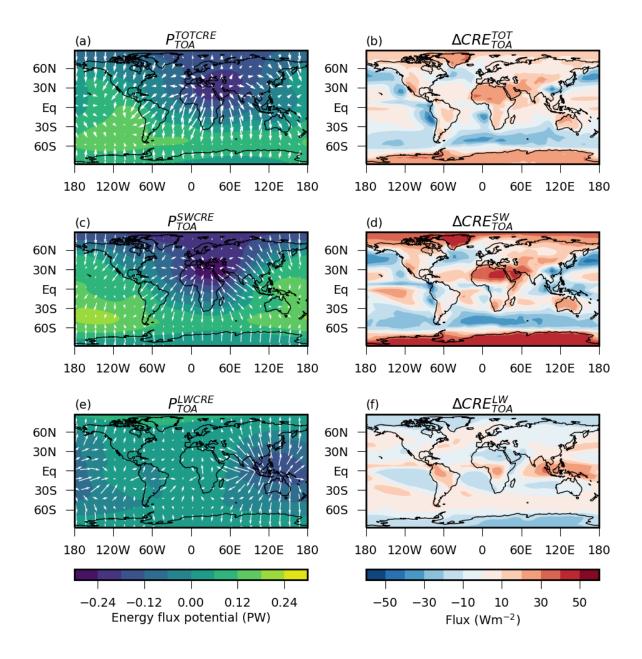


Fig. 40: As in Fig. 38, but for the implied heat transport associated with (a),(b) TOT CRE, (c),(d) SW CRE, and (e),(f) LW CRE fluxes.

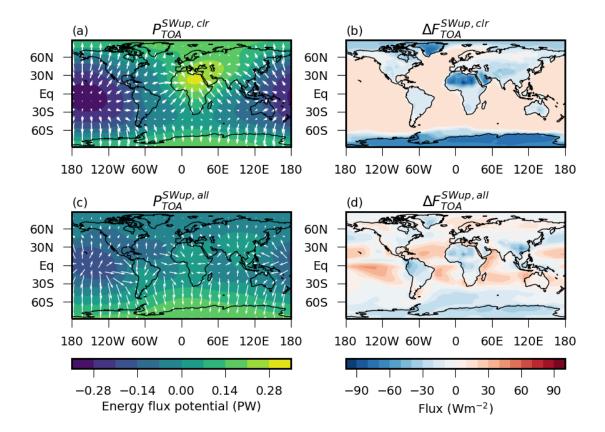


Fig. 41: As in Fig. 38, but for (a), (b) clear-sky and (c), (d) all-sky reflected SW flux.

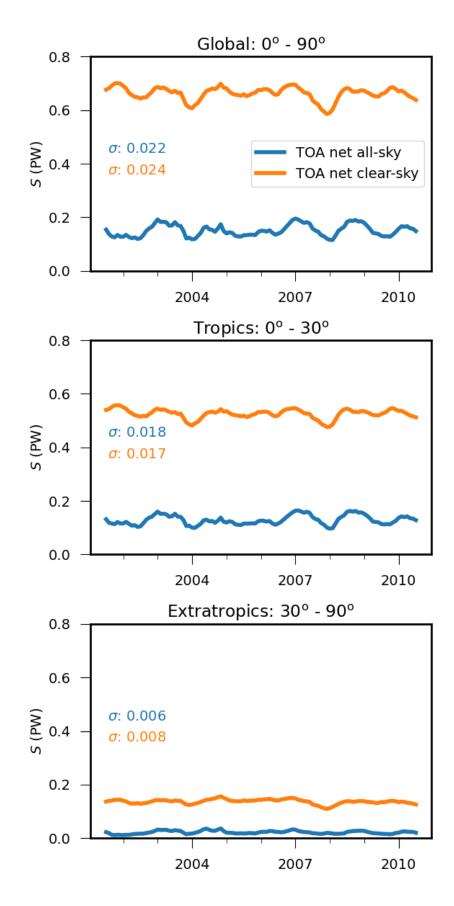


Fig. 42: A measure of the symmetry between heat transport in the Northern and Southern Hemispheres, calculated **15.17**. 1 **Phick insights for climate impact researchers** (a) the full hemisphere, (b) from the equator to 30°, and (c) 30° to 90°. Symmetry values obtained when including (blue) and excluding (orange) the effect of clouds. The climatological symmetry values for the two cases are shown as the black lines in each subplot, dashed and dotted, respectively. The standard deviations of the time series are shown in each plot.

#### 15.17.6 References

• None

## 15.17.7 Example plots

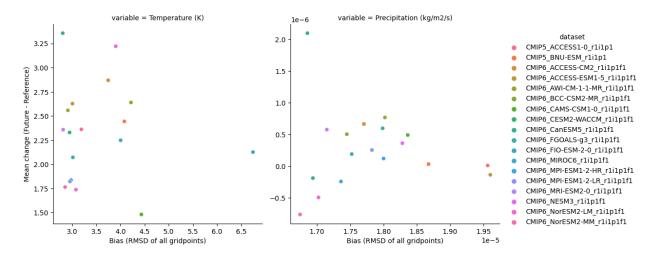


Fig. 43: "Bias and change for each variable"

## 15.18 Modes of variability

#### 15.18.1 Overview

The goal of this recipe is to compute modes of variability from a reference or observational dataset and from a set of climate projections and calculate the root-mean-square error between the mean anomalies obtained for the clusters from the reference and projection data sets. This is done through K-means or hierarchical clustering applied either directly to the spatial data or after computing the EOFs.

The user can specify the number of clusters to be computed.

The recipe's output consist of three netcdf files for both the observed and projected weather regimes and the RMSE between them.

## 15.18.2 Available recipes and diagnostics

Recipes are stored in recipes/

recipe\_modes\_of\_variability.yml

Diagnostics are stored in diag\_scripts/magic\_bsc/

- WeatherRegime.R function for computing the EOFs and k-means and hierarchical clusters.
- weather\_regime.R applies the above weather regimes function to the datasets

#### 15.18.3 User settings

User setting files are stored in recipes/

1. recipe\_modes\_of\_variability.yml

Required settings for script

- plot type: rectangular or polar
- ncenters: number of centers to be computed by the clustering algorithm (maximum 4)
- cluster\_method: kmeans (only psl variable) or hierarchical clustering (for psl or sic variables)
- detrend\_order: the order of the polynomial detrending to be applied (0, 1 or 2)
- EOFs: logical indicating wether the k-means clustering algorithm is applied directly to the spatial data ('false') or to the EOFs ('true')
- frequency: select the month (format: JAN, FEB, ...) or season (format: JJA, SON, MAM, DJF) for the diagnostic to be computed for (does not work yet for MAM with daily data).

## 15.18.4 Variables

• psl (atmos, monthly/daily, longitude, latitude, time)

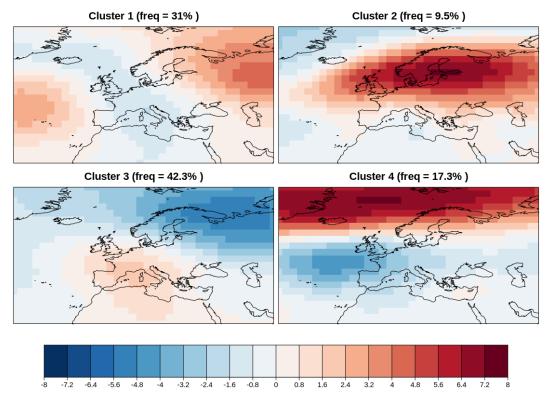
## 15.18.5 Observations and reformat scripts

None

## 15.18.6 References

- Dawson, A., T. N. Palmer, and S. Corti, 2012: Simulating regime structures in weather and climate prediction models. Geophysical Research Letters, 39 (21), https://doi.org/10.1029/2012GL053284.
- Ferranti, L., S. Corti, and M. Janousek, 2015: Flow-dependent verification of the ECMWF ensemble over the Euro-Atlantic sector. Quarterly Journal of the Royal Meteorological Society, 141 (688), 916-924, https://doi.org/10.1002/qj.2411.
- Grams, C. M., Beerli, R., Pfenninger, S., Staffell, I., & Wernli, H. (2017). Balancing Europe's wind-power output through spatial deployment informed by weather regimes. Nature climate change, 7(8), 557, https://doi.org/10. 1038/nclimate3338.
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## 15.18.7 Example plots



Four modes of variability for autumn (September-October-November) in the North Atlantic European Sector for the RCP 8.5 scenario using BCC-CSM1-1 future projection during the period 2020-2075. The frequency of occurrence of each variability mode is indicated in the title of each map.

# 15.19 Diagnostics of integrated atmospheric methane (XCH4)

## 15.19.1 Overview

This recipe <u>recipe\_mpqb\_xch4.yml</u> allows the comparison of integrated atmospheric methane between CMIP6 model simulations and observations, and produces lineplots of monthly mean methane values, annual cycles and annual growth rates:

- Monthly mean time series of XCH4 for pre-defined regions (global, Northern Hemisphere, Southern Hemisphere)
- Annual cycles of XCH4 for pre-defined regions (global, Northern Hemisphere, Southern Hemisphere)
- Annual growth rates of XCH4 for pre-defined regions (global, Northern Hemisphere, Southern Hemisphere)

#### 15.19.2 Available recipes and diagnostics

Recipes are stored in esmvaltool/recipes/mpqb/

• recipe\_mpqb\_xch4.yml

Diagnostics are stored in esmvaltool/diag\_scripts/mpqb/

- mpqb\_lineplot.py
- mpqb\_lineplot\_anncyc.py
- mpqb\_lineplot\_growthrate.py

## 15.19.3 Observations and reformat scripts

Observations used in this recipe are:

• CDS-XCH4 (ESA CCI dataset served on the Copernicus Climate data store)

A cmorizing script for this dataset is available (cmorize\_obs\_cds\_xch4.ncl).

XCH4 is a derived variable that needs to be calculated from four different variables (ch4, hus, zg, ps). A derivation script is included in the ESMValCore.

## 15.19.4 User settings in recipe

- 1. Preprocessor
  - pp\_lineplots\_xx\_mon: Regridding, masking all missing values from all used datasets, area-mean ('xx' can ge replaced by 'gl'=global, 'sh'=southern hemisphere, 'nh'=northern hemisphere), units converted to [ppbv] to obtain one time series of monthly mean values for the selected region (global, southern hemisphere, northern hemisphere)
  - pp\_lineplots\_xx\_ann: Regridding, masking all missing values from all used datasets, area-mean ('xx' can ge replaced by 'gl'=global, 'sh'=southern hemisphere, 'nh'=northern hemisphere), units converted to [ppbv] to obtain one time series of annual mean values for the selected region (global, southern hemisphere, northern hemisphere)
  - pp\_lineplots\_anncyc\_xx: : Regridding, masking all missing values from all used datasets, area-mean ('xx' can ge replaced by 'gl'=global, 'sh'=southern hemisphere, 'nh'=northern hemisphere), units converted to [ppbv], monthly climate statistics applied to one annual cycle for the whole chosen time period and for the selected region (global, southern hemisphere, northern hemisphere)
  - xch4\_def\_xx: defining the time period over which the analysis should be calculated; options are "cmip6" which overlapping period of the observations and the CMIP6 historical simulations, and "future" which covers the time period of CMIP6 scenarios
- 2. Additional needed files
  - mpqb\_cfg\_xch4.yml: In this file additional information for the used datasets are defined and stored, e.g. alias of the dataset name and the color that is used to display the dataset in the figures
  - mpqb\_utils.yml: In this file the preparations for the dataset displays are made.
- 3. Script <mpqb\_lineplot.py>

Required settings for script

• no additional settings required

Optional settings for script

- no optional settings available
- Required settings for variables
  - no settings for the variable required
- 4. Script <mpqb\_lineplot\_anncyc.py>
  - Required settings for script
    - no additional settings required
  - Optional settings for script
    - no optional settings available
  - Required settings for variables
    - no settings for the variable required
- 5. Script <mpqb\_lineplot\_growthrate.py>
  - Required settings for script
    - no additional settings required
  - Optional settings for script
    - no optional settings available

Required settings for variables

• no settings for the variable required

## 15.19.5 Variables

- ch4 (atmos, monthly mean, longitude latitude level time)
- hus (atmos, monthly mean, longitude latitude level time)
- zg (atmos, monthly mean, longitude latitude level time)
- ps (atmos, monthly mean, longitude latitude time)

All variables are necessary to calculate the derived variable xch4.

## 15.19.6 Example plots

# 15.20 Precipitation quantile bias

## 15.20.1 Overview

Precipitation is a dominant component of the hydrological cycle, and as such a main driver of the climate system and human development. The reliability of climate projections and water resources strategies therefore depends on how well precipitation can be reproduced by the models used for simulations. While global circulation models from the CMIP5 project observations can reproduce the main patterns of mean precipitation, they often show shortages and biases in the ability to reproduce the strong precipitation tails of the distribution. Most models underestimate precipitation over arid regions and overestimate it over regions of complex topography, and these shortages are amplified at high quantile precipitation. The quantilebias recipe implements calculation of the quantile bias to allow evaluation of the precipitation bias based on a user defined quantile in models as compared to a reference dataset following Mehran et al. (2014). The quantile bias (QB) is defined as the ratio of monthly precipitation amounts in each simulation to that of the

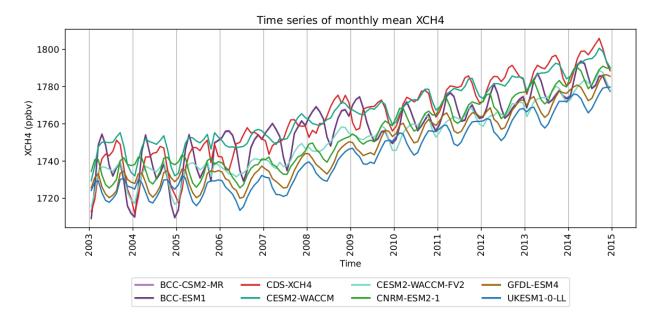


Fig. 44: Monthly mean time series of XCH4, calculated over the whole globe, for individual CMIP6 model simulations.

reference dataset (GPCP observations in the example) above a specified threshold t (e.g., the 75th percentile of all the local monthly values). A quantile bias equal to 1 indicates no bias in the simulations, whereas a value above (below) 1 corresponds to a climate model's overestimation (underestimation) of the precipitation amount above the specified threshold t, with respect to that of the reference dataset.

## 15.20.2 Available recipes and diagnostics

Recipes are stored in recipes/

recipe\_quantilebias.yml

Diagnostics are stored in diag\_scripts/quantilebias/

• quantilebias.R

## 15.20.3 User settings

Required settings for script

• perc\_lev: quantile (in %), e.g. 50

## 15.20.4 Variables

• pr (atmos, monthly, longitude latitude time)

#### 15.20.5 Observations and reformat scripts

• GPCP-SG observations (accessible via the obs4MIPs project)

#### 15.20.6 References

• Mehran, A. et al.: Journal of Geophysical Research: Atmospheres, Volume 119, Issue 4, pp. 1695-1707, 2014.

## 15.20.7 Example plots

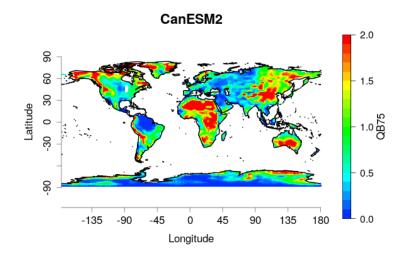


Fig. 45: Quantile bias, as defined in Mehran et al. 2014, with threshold t=75th percentile, evaluated for the CanESM2 model over the 1979-2005 period, adopting GPCP-SG v 2.3 gridded precipitation as a reference dataset. The optimal reference value is 1. Both datasets have been regridded onto a  $2^{\circ}$  regular grid.

# **15.21 Quantifying progress across different CMIP phases**

## 15.21.1 Overview

The recipe recipe\_bock20jgr.yml generates figures to quantify the progress across different CMIP phases.

**Note:** The current recipe uses a horizontal 5x5 grid for figure 10, while the original plot in the paper shows a 2x2 grid. This is solely done for computational reasons (running the recipe with a 2x2 grid for figure 10 takes considerably more time than running it with a 5x5 grid) and can be easily changed in the preprocessor section of the recipe if necessary.

#### 15.21.2 Available recipes and diagnostics

Recipes are stored in recipes/bock20jgr

- recipe\_bock20jgr\_fig\_1-4.yml
- recipe\_bock20jgr\_fig\_6-7.yml
- recipe\_bock20jgr\_fig\_8-10.yml

Diagnostics are stored in diag\_scripts/

Fig. 1:

• bock20jgr/tsline.ncl: timeseries of global mean surface temperature anomalies

Fig. 2:

• bock20jgr/tsline\_collect.ncl: collect different timeseries from tsline.ncl to compare different models ensembles

Fig. 3 and 4:

• bock20jgr/model\_bias.ncl: global maps of the multi-model mean and the multi-model mean bias

Fig. 6:

- perfmetrics/main.ncl
- perfmetrics/collect.ncl

Fig. 7:

- bock20jgr/corr\_pattern.ncl: calculate pattern correlation
- bock20jgr/corr\_pattern\_collect.ncl: create pattern correlation plot

Fig. 8:

- climate\_metrics/ecs.py
- climate\_metrics/create\_barplot.py

Fig. 9:

clouds/clouds\_ipcc.ncl

Fig. 10:

climate\_metrics/feedback\_parameters.py

#### 15.21.3 User settings in recipe

1. Script tsline.ncl

Required settings (scripts)

• styleset: as in diag\_scripts/shared/plot/style.ncl functions

Optional settings (scripts)

- time\_avg: type of time average (currently only "yearly" and "monthly" are available).
- ts\_anomaly: calculates anomalies with respect to the defined reference period; for each grid point by removing the mean for the given calendar month (requiring at least 50% of the data to be non-missing)
- ref\_start: start year of reference period for anomalies

- ref\_end: end year of reference period for anomalies
- ref\_value: if true, right panel with mean values is attached
- ref\_mask: if true, model fields will be masked by reference fields
- region: name of domain
- plot\_units: variable unit for plotting
- y\_min: set min of y-axis
- y\_max: set max of y-axis
- mean\_nh\_sh: if true, calculate first NH and SH mean
- volcanoes: if true, lines of main volcanic eruptions will be added
- header: if true, use region name as header
- write\_stat: if true, write multi-model statistics to nc-file

#### Required settings (variables)

none

• Optional settings (variables)

none

2. Script tsline\_collect.ncl

Required settings (scripts)

• styleset: as in diag\_scripts/shared/plot/style.ncl functions

**Optional settings (scripts)** 

- time\_avg: type of time average (currently only "yearly" and "monthly" are available).
- ts\_anomaly: calculates anomalies with respect to the defined period
- ref\_start: start year of reference period for anomalies
- ref\_end: end year of reference period for anomalies
- region: name of domain
- plot\_units: variable unit for plotting
- y\_min: set min of y-axis
- y\_max: set max of y-axis
- order: order in which experiments should be plotted
- header: if true, region name as header
- stat\_shading: if true: shading of statistic range
- ref\_shading: if true: shading of reference period

Required settings (variables)

none

• Optional settings (variables)

none

3. Script model\_bias.ncl

```
Required settings (scripts)
```

none

Optional settings (scripts)

- projection: map projection, e.g., Mollweide, Mercator
- timemean: time averaging, i.e. "seasonalclim" (DJF, MAM, JJA, SON), "annualclim" (annual mean)
- Required settings (variables)\*
- reference\_dataset: name of reference dataset

Optional settings (variables)

long\_name: description of variable

Color tables

- variable "tas": diag\_scripts/shared/plot/rgb/ipcc-ar6\_temperature\_div.rgb,
- variable "pr-mmday": diag\_scripts/shared/plots/rgb/ipcc-ar6\_precipitation\_seq.rgb diag\_scripts/shared/plot/rgb/ipcc-ar6\_precipitation\_div.rgb

4. Script perfmetrics\_main.ncl

See here.

5. Script perfmetrics\_collect.ncl

See *here*.

6. Script corr\_pattern.ncl

Required settings (scripts)

none

**Optional settings (scripts)** 

• plot\_median

Required settings (variables)

reference\_dataset

Optional settings (variables)

- alternative\_dataset
- 7. Script corr\_pattern\_collect.ncl

Required settings (scripts)

none

Optional settings (scripts)

diag\_order

Color tables

- diag\_scripts/shared/plot/rgb/ipcc-ar6\_line\_03.rgb
- 8. Script ecs.py

See here.

9. Script create\_barplot.py

See *here*.

10. Script clouds\_ipcc.ncl

See here.

11. Script feedback\_parameters.py

Required settings (scripts)

none

Optional settings (scripts)

- calculate\_mmm: bool (default: True). Calculate multi-model means.
- only\_consider\_mmm: *bool* (default: False). Only consider multi-model mean dataset. This automatically sets calculate\_mmm to True. For large multi-dimensional datasets, this might significantly reduce the computation time if only the multi-model mean dataset is relevant.
- output\_attributes: dict. Write additional attributes to netcdf files.
- seaborn\_settings: *dict*. Options for seaborn.set\_theme() (affects all plots).

## 15.21.4 Variables

- clt (atmos, monthly, longitude latitude time)
- hus (atmos, monthly, longitude latitude lev time)
- pr (atmos, monthly, longitude latitude time)
- psl (atmos, monthly, longitude latitude time)
- rlut (atmos, monthly, longitude latitude time)
- rsdt (atmos, monthly, longitude latitude time)
- rsut (atmos, monthly, longitude latitude time)
- rtmt (atmos, monthly, longitude latitude time)
- rlutcs (atmos, monthly, longitude latitude time)
- rsutcs (atmos, monthly, longitude latitude time)
- ta (atmos, monthly, longitude latitude lev time)
- tas (atmos, monthly, longitude latitude time)
- ts (atmos, monthly, longitude latitude time)
- ua (atmos, monthly, longitude latitude lev time)
- va (atmos, monthly, longitude latitude lev time)
- zg (atmos, monthly, longitude latitude time)

#### 15.21.5 Observations and reformat scripts

- AIRS (obs4MIPs) specific humidity
- CERES-EBAF (obs4MIPs) CERES TOA radiation fluxes (used for calculation of cloud forcing)
- ERA-Interim reanalysis of surface temperature, sea surface pressure *Reformat script:* recipes/cmorizers/recipe\_era5.yml
- ERA5 reanalysis of surface temperature

Reformat script: recipes/cmorizers/recipe\_era5.yml

• ESACCI-CLOUD - total cloud cover

Reformat script: cmorizers/data/formatters/datasets/esacci\_cloud.ncl

- ESACCI-SST sea surface temperature
- Reformat script: cmorizers/data/formatters/datasets/esacci\_sst.py
- GHCN Global Historical Climatology Network-Monthly gridded land precipitation *Reformat script:* cmorizers/data/formatters/datasets/ghcn.ncl
- GPCP-SG (obs4MIPs) Global Precipitation Climatology Project total precipitation
- HadCRUT4 surface temperature anomalies

Reformat script: cmorizers/data/formatters/datasets/hadcrut4.ncl

• HadISST - surface temperature

Reformat script: cmorizers/data/formatters/datasets/hadisst.ncl

- JRA-55 (ana4mips) reanalysis of sea surface pressure
- NCEP-NCAR-R1 reanalysis of surface temperature

Reformat script: cmorizers/data/formatters/datasets/ncep\_ncar\_r1.py

• PATMOS-x - total cloud cover

Reformat script: cmorizers/data/formatters/datasets/patmos\_x.ncl

## 15.21.6 References

- Bock, L., Lauer, A., Schlund, M., Barreiro, M., Bellouin, N., Jones, C., Predoi, V., Meehl, G., Roberts, M., and Eyring, V.: Quantifying progress across different CMIP phases with the ESMValTool, Journal of Geophysical Research: Atmospheres, 125, e2019JD032321. https://doi.org/10.1029/2019JD032321
- Copernicus Climate Change Service (C3S), 2017: ERA5: Fifth generation of ECMWF atmospheric reanalyses of the global climate, edited, Copernicus Climate Change Service Climate Data Store (CDS). https://cds.climate.copernicus.eu/cdsapp#!/home
- Flato, G., J. Marotzke, B. Abiodun, P. Braconnot, S.C. Chou, W. Collins, P. Cox, F. Driouech, S. Emori, V. Eyring, C. Forest, P. Gleckler, E. Guilyardi, C. Jakob, V. Kattsov, C. Reason and M. Rummukainen, 2013: Evaluation of Climate Models. In: Climate Change 2013: The Physical Science Basis. Contribution of Working Group I to the Fifth Assessment Report of the Intergovernmental Panel on Climate Change [Stocker, T.F., D. Qin, G.-K. Plattner, M. Tignor, S.K. Allen, J. Boschung, A. Nauels, Y. Xia, V. Bex and P.M. Midgley (eds.)]. Cambridge University Press, Cambridge, United Kingdom and New York, NY, USA.

 Morice, C. P., Kennedy, J. J., Rayner, N. A., & Jones, P., 2012: Quantifying uncertainties in global and regional temperature change using an ensemble of observational estimates: The HadCRUT4 data set, Journal of Geophysical Research, 117, D08101. https://doi.org/10.1029/2011JD017187

## 15.21.7 Example plots

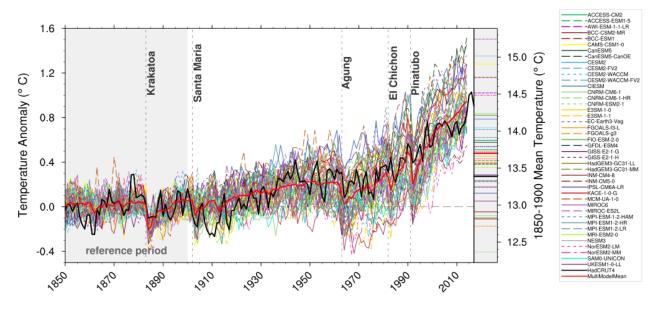


Fig. 46: Observed and simulated time series of the anomalies in annual and global mean surface temperature. All anomalies are differences from the 1850-1900 time mean of each individual time series (Fig. 1).

# 15.22 Standardized Precipitation-Evapotranspiration Index (SPEI)

## 15.22.1 Overview

Droughts can be separated into three main types: meteorological, hydrological, and agricultural drought.

Common for all types is that a drought needs to be put in context of local and seasonal characteristics, i.e. a drought should not be defined with an absolute threshold, but as an anomalous condition.

Meteorological droughts are often described using the standardized precipitation index (SPI; McKee et al, 1993), which in a standardized way describes local precipitation anomalies. It is calculated on monthly mean precipitation, and is therefore not accounting for the intensity of precipitation and the runoff process. Because SPI does not account for evaporation from the ground, it lacks one component of the water fluxes at the surface and is therefore not compatible with the concept of hydrological drought.

A hydrological drought occurs when low water supply becomes evident, especially in streams, reservoirs, and groundwater levels, usually after extended periods of meteorological drought. GCMs normally do not simulate hydrological processes in sufficient detail to give deeper insights into hydrological drought processes. Neither do they properly describe agricultural droughts, when crops become affected by the hydrological drought. However, hydrological drought can be estimated by accounting for evapotranspiration, and thereby estimate the surface retention of water. The standardized precipitation-evapotranspiration index (SPEI; Vicente-Serrano et al., 2010) has been developed to also account for temperature effects on the surface water fluxes. Evapotranspiration is not normally calculated in GCMs, so SPEI often takes other inputs to estimate the evapotranspiration. Here, the Thornthwaite (Thornthwaite, 1948) method based on temperature is applied.

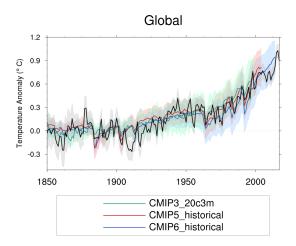


Fig. 47: Observed and simulated time series of the anomalies in annual and global mean surface temperature as in Figure 1; all anomalies are calculated by subtracting the 1850-1900 time mean from the time series. Displayed are the multimodel means of all three CMIP ensembles with shaded range of the respective standard deviation. In black the HadCRUT4 data set (HadCRUT4; Morice et al., 2012). Gray shading shows the 5% to 95% confidence interval of the combined effects of all the uncertainties described in the HadCRUT4 error model (measurement and sampling, bias, and coverage uncertainties) (Morice et al., 2012) (Fig. 2).

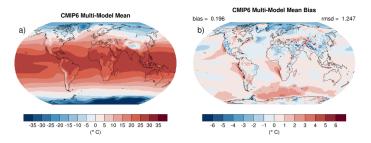


Fig. 48: Annual mean near-surface (2 m) air temperature (°C). (a) Multimodel (ensemble) mean constructed with one realization of CMIP6 historical experiments for the period 1995-2014. Multimodel-mean bias of (b) CMIP6 (1995-2014) compared to the corresponding time period of the climatology from ERA5 (Copernicus Climate Change Service (C3S), 2017). (Fig. 3)

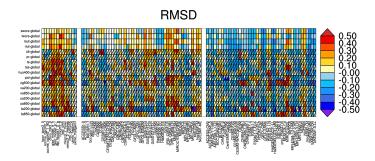


Fig. 49: Relative space-time root-mean-square deviation (RMSD) calculated from the climatological seasonal cycle of the CMIP3, CMIP5, and CMIP6 simulations (1980-1999) compared to observational data sets (Table 5). A relative performance is displayed, with blue shading being better and red shading worse than the median RMSD of all model results of all ensembles. A diagonal split of a grid square shows the relative error with respect to the reference data set (lower right triangle) and the alternative data set (upper left triangle) which are marked in Table 5. White boxes are used when data are not available for a given model and variable (Fig. 6).

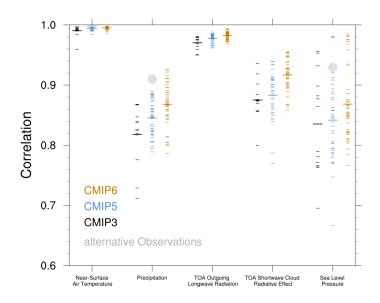


Fig. 50: Centered pattern correlations between models and observations for the annual mean climatology over the period 1980–1999 (Fig. 7).

## 15.22.2 Available recipes and diagnostics

Recipes are stored in recipes/

recipe\_spei.yml

Diagnostics are stored in diag\_scripts/droughtindex/

- diag\_spi.R: calculate the SPI index
- diag\_spei.R: calculate the SPEI index

## 15.22.3 User settings

1. Script diag\_spi.py

Required settings (script)

- reference\_dataset: dataset\_name The reference data set acts as a baseline for calculating model bias.
- 2. Script diag\_spei.py

Required settings (script)

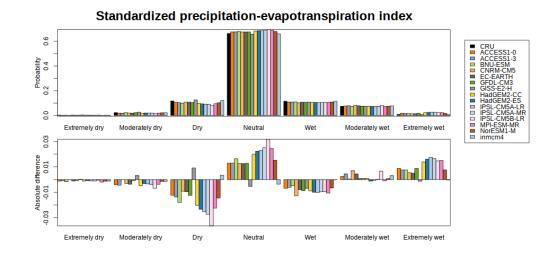
• reference\_dataset: dataset\_name The reference data set acts as a baseline for calculating model bias.

#### 15.22.4 Variables

- pr (atmos, monthly mean, time latitude longitude)
- tas (atmos, monthly mean, time latitude longitude)

#### 15.22.5 References

- McKee, T. B., Doesken, N. J., & Kleist, J. (1993). The relationship of drought frequency and duration to time scales. In Proceedings of the 8th Conference on Applied Climatology (Vol. 17, No. 22, pp. 179-183). Boston, MA: American Meteorological Society.
- Vicente-Serrano, S. M., Beguería, S., & López-Moreno, J. I. (2010). A multiscalar drought index sensitive to global warming: the standardized precipitation evapotranspiration index. Journal of climate, 23(7), 1696-1718.



## 15.22.6 Example plots

Fig. 51: (top) Probability distribution of the standardized precipitation-evapotranspiration index of a sub-set of the CMIP5 models, and (bottom) bias relative to the CRU reference data set.

# 15.23 Drought characteristics following Martin (2018)

## 15.23.1 Overview

Following Martin (2018) drought characteristics are calculated based on the standard precipitation index (SPI), see Mckee et al. (1993). These characteristics are frequency, average duration, SPI index and severity index of drought events.

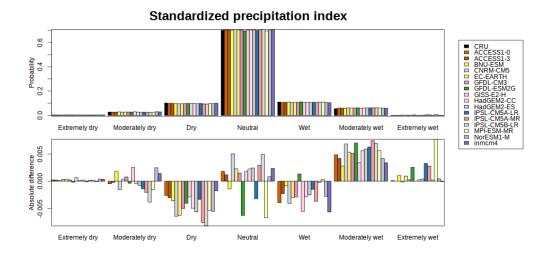


Fig. 52: (top) Probability distribution of the standardized precipitation index of a sub-set of the CMIP5 models, and (bottom) bias relative to the CRU reference data set.

## 15.23.2 Available recipes and diagnostics

Recipes are stored in recipes/

• recipe\_martin18grl.yml

Diagnostics are stored in diag\_scripts/

- droughtindex/diag\_save\_spi.R
- droughtindex/collect\_drought\_obs\_multi.py
- droughtindex/collect\_drought\_model.py
- droughtindex/collect\_drought\_func.py

## 15.23.3 User settings in recipe

The recipe can be run with different CMIP5 and CMIP6 models and one observational or reanalysis data set.

The droughtindex/diag\_save\_spi.R script calculates the SPI index for any given time series. It is based on droughtindex/diag\_spi.R but saves the SPI index and does not plot the histogram. The distribution and the representative time scale (smooth\_month) can be set by the user, the values used in Martin (2018) are smooth\_month: 6 and distribution: 'Gamma' for SPI.

There are two python diagnostics, which can use the SPI data to calculate the drought characteristics (frequency, average duration, SPI index and severity index of drought events) based on Martin (2018):

- To compare these characteristics between model data and observations or renanalysis data use droughtin-dex/collect\_drought\_obs\_multi.py Here, the user can set: \* indexname: Necessary to identify data produced by droughtindex/diag\_save\_spi.R as well as write captions and filenames. At the moment only indexname: 'SPI' is supported. \* threshold: Threshold for this index below which an event is considered to be a drought, the setting for SPI should be usually threshold: -2.0 but any other value will be accepted. Values should not be < 3.0 or > 3.0 for SPI (else it will identify none/always drought conditions).
- To compare these ccharacteristics between different time periods in model data use droughtindex/collect\_drought\_model.py Here, the user can set: \* indexname: Necessary to identify data produced

by droughtindex/diag\_save\_spi.R as well as write captions and filenames. At the moment only indexname: 'SPI' is supported. \* threshold: Threshold for this index below which an event is considered to be a drought, the setting for SPI should be usually threshold: -2.0 but any other value will be accepted. Values should not be < - 3.0 or > 3.0 for SPI (else it will identify none/always drought conditions). \* start\_year: Needs to be equal or larger than the start\_year for droughtindex/diag\_save\_spi.R. \* end\_year: Needs to be equal or smaller than the end\_year for droughtindex/diag\_save\_spi.R. \* comparison\_period: should be < (end\_year - start\_year)/2 to have non overlapping time series in the comparison.

The third diagnostic droughtindex/collect\_drought\_func.py contains functions both ones above use.

#### 15.23.4 Variables

• pr (atmos, monthly, longitude, latitude, time)

#### 15.23.5 Observations and reformat scripts

None

#### 15.23.6 References

- Martin, E.R. (2018). Future Projections of Global Pluvial and Drought Event Characteristics. Geophysical Research Letters, 45, 11913-11920.
- McKee, T. B., Doesken, N. J., & Kleist, J. (1993). The relationship of drought frequency and duration to time scales. In Proceedings of the 8th Conference on Applied Climatology (Vol. 17, No. 22, pp. 179-183). Boston, MA: American Meteorological Society.

#### 15.23.7 Example plots

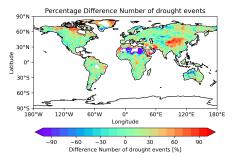


Fig. 53: Global map of the percentage difference between multi-model mean of 15 CMIP models and the CRU data for the number of drought events [%] based on SPI.

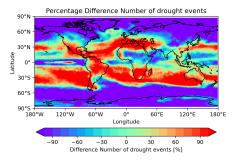


Fig. 54: Global map of the percentage difference between multi-model mean for RCP8.5 scenarios (2050-2100) runs and historical data (1950-2000) for 15 CMIP models for the number of drought events [%] based on SPI.

# 15.24 Stratosphere - Autoassess diagnostics

#### 15.24.1 Overview

Polar night jet / easterly jet strengths are defined as the maximum / minimum wind speed of the climatological zonal mean jet, and measure how realistic the zonal wind climatology is in the stratosphere.

Extratropical temperature at 50hPa (area averaged poleward of 60 degrees) is important for polar stratospheric cloud formation (in winter/spring), determining the amount of heterogeneous ozone depletion simulated by models with interactive chemistry schemes.

The Quasi-Biennial Oscillation (QBO) is a good measure of tropical variability in the stratosphere. Zonal mean zonal wind at 30hPa is used to define the period and amplitude of the QBO.

The tropical tropopause cold point (100hPa, 10S-10N) temperature is an important factor in determining the stratospheric water vapour concentrations at entry point (70hPa, 10S-10N), and this in turn is important for the accurate simulation of stratospheric chemistry and radiative balance.

Performance metrics:

- Polar night jet: northern hem (January) vs. ERA Interim
- Polar night jet: southern hem (July) vs. ERA Interim
- Easterly jet: southern hem (January) vs. ERA Interim
- Easterly jet: northern hem (July) vs. ERA Interim
- 50 hPa temperature: 60N-90N (DJF) vs. ERA Interim
- 50 hPa temperature: 60N-90N (MAM) vs. ERA Interim
- 50 hPa temperature: 90S-60S (JJA) vs. ERA Interim
- 50 hPa temperature: 90S-60S (SON) vs. ERA Interim
- QBO period at 30 hPa vs. ERA Interim
- QBO amplitude at 30 hPa (westward) vs. ERA Interim
- QBO amplitude at 30 hPa (eastward) vs. ERA Interim
- 100 hPa equatorial temp (annual mean) vs. ERA Interim
- 100 hPa equatorial temp (annual cycle strength) vs. ERA Interim
- 70 hPa 10S-10N water vapour (annual mean) vs. ERA-Interim

Diagnostic plot:

• Age of stratospheric air vs. observations from Andrews et al. (2001) and Engel et al. (2009)

#### 15.24.2 Available recipes and diagnostics

Recipes are stored in esmvaltool/recipes/

recipe\_autoassess\_stratosphere.yml

Diagnostics are stored in esmvaltool/diag\_scripts/autoassess/

- autoassess\_area\_base.py: wrapper for autoassess scripts
- stratosphere/strat\_metrics\_1.py: calculation of metrics
- stratosphere/age\_of\_air.py: calculate age of stratospheric air
- stratosphere/plotting.py: zonal mean wind and QBO plots
- plot\_autoassess\_metrics.py: plot normalised assessment metrics

#### 15.24.3 User settings in recipe

The stratosphere area metric is part of the esmvaltool/diag\_scripts/autoassess diagnostics, and, as any other autoassess metric, it uses the autoassess\_area\_base.py as general purpose wrapper. This wrapper accepts a number of input arguments that are read through from the recipe.

This recipe is part of the larger group of Autoassess metrics ported to ESMValTool from the native Autoassess package from the UK's Met Office. The diagnostics settings are almost the same as for the other Atoassess metrics.

#### Note: Time gating for autoassess metrics.

To preserve the native Autoassess functionalities, data loading and selection on time is done somewhat differently for ESMValTool's autoassess metrics: the time selection is done in the preprocessor as per usual but a further time selection is performed as part of the diagnostic. For this purpose the user will specify a start: and end: pair of arguments of scripts: autoassess\_script (see below for example). These are formatted as YYYY/MM/DD; this is necessary since the Autoassess metrics are computed from 1-Dec through 1-Dec rather than 1-Jan through 1-Jan. This is a temporary implementation to fully replicate the native Autoassess functionality and a minor user inconvenience since they need to set an extra set of start and end arguments in the diagnostic; this will be phased when all the native Autoassess metrics have been ported to ESMValTool review has completed.

#### Note: Polar Night/Easterly Jets Metrics

Polar Night Jets (PNJ) metrics require data available at very low air pressures ie very high altitudes; both Olar Night Jet and Easterly Jets computations should be preformed using ta and ua data at << 100 Pa; the lowest air pressure found in atmospheric CMOR mip tables corresponds to plev39 air pressure table, and is used in the AERmonZ mip. If the user requires correct calculations of these jets, it is highly advisable to use data from AERmonZ. Note that standard QBO calculation is exact for plev19 tables.

An example of standard inputs as read by autoassess\_area\_base.py and passed over to the diagnostic/metric is listed below.

scripts:
<pre>autoassess_strato_test_1: &amp;autoassess_strato_test_1_settings</pre>
<pre>script: autoassess/autoassess_area_base.py # the base wrapper</pre>
<pre>title: "Autoassess Stratosphere Diagnostic Metric" # title</pre>
<b>area</b> : stratosphere <i># assesment area</i>
<pre>control_model: UKESM1-0-LL-hist # control dataset name</pre>
<pre>exp_model: UKESM1-0-LL-piCont # experiment dataset name</pre>
obs_models: [ERA-Interim] # list to hold models that are NOT for metrics but for
⇔obs operations
additional_metrics: [ERA-Interim] # list to hold additional datasets for metrics
<pre>start: 2004/12/01 # start date in native Autoassess format</pre>
<pre>end: 2014/12/01 # end date in native Autoassess format</pre>

#### 15.24.4 Variables

Variable/Field name	realm	frequency	Comment
Eastward wind (ua)	Atmosphere	monthly mean	original stash: x-wind, no stash
Air temperature (ta)	Atmosphere	monthly mean	original stash: m01s30i204
Specific humidity (hus)	Atmosphere	monthly mean	original stash: m01s30i205

The recipe takes as input a control model and experimental model, comparisons being made with these two CMIP models; additionally it can take observational data s input, in the current implementation ERA-Interim.

#### 15.24.5 Observations and reformat scripts

ERA-Interim (ta, ua, hus - cmorizers/data/formatters/datasets/era\_interim.py)

#### 15.24.6 References

- Andrews, A. E., and Coauthors, 2001: Mean ages of stratospheric air derived from in situ observations of CO2, CH4, and N2O. J. Geophys. Res., 106 (D23), 32295-32314.
- Dee, D. P., and Coauthors, 2011: The ERA-Interim reanalysis: configuration and performance of the data assimilation system. Q. J. R. Meteorol. Soc, 137, 553-597, doi:10.1002/qj.828.
- Engel, A., and Coauthors, 2009: Age of stratospheric air unchanged within uncertainties over the past 30 years. Nat. Geosci., 2, 28-31, doi:10.1038/NGEO388.

#### 15.24.7 Example metrics and plots

Below is a set of metrics for UKESM1-0-LL (historical data); the table shows a comparison made between running ESMValTool on CMIP6 CMORized netCDF data freely available on ESGF nodes and the run made using native Autoassess performed at the Met Office using the pp output of the model.

Metric name	UKESM1-0-LL; CMIP6: historical, ESGF	AERmonZ;	UKESM1-0-LL; pp files; histor- ical, u-bc179
Polar night jet: northern hem (Jan- uary)	44.86		44.91
Polar night jet: southern hem (July)	112.09		112.05
Easterly jet: southern hem (Jan- uary)	76.12		75.85
Easterly jet: northern hem (July)	55.68		55.74
QBO period at 30 hPa	41.50		41.00
QBO amplitude at 30 hPa (west-ward)	27.39		27.39
QBO amplitude at 30 hPa (east-ward)	17.36		17.36
50 hPa temperature: 60N-90N (DJF)	27.11		26.85
50 hPa temperature: 60N-90N (MAM)	40.94		40.92
50 hPa temperature: 90S-60S (JJA)	11.75		11.30
50 hPa temperature: 90S-60S (SON)	23.88		23.63
100 hPa equatorial temp (annual mean)	15.29		15.30
100 hPa equatorial temp (annual cycle strength)	1.67		1.67
100 hPa 10Sto10N temp (annual mean)	15.48		15.46
100 hPa 10Sto10N temp (annual cycle strength)	1.62		1.62
70 hPa 10Sto10N wv (annual mean)	5.75		5.75

Results from u-bc179 have been obtained by running the native Autoassess/stratosphere on .pp data from UKESM1 u-bc179 suite and are listed here to confirm the compliance between the ported Autoassess metric in ESMValTool and the original native metric.

Another reference run comparing UKESM1-0-LL to the physical model HadGEM3-GC31-LL can be found here .

#### 15.24.8 Prior and current contributors

Met Office:

- Prior to May 2008: Neal Butchart
- May 2008 May 2016: Steven C Hardiman
- Since May 2016: Alistair Sellar and Paul Earnshaw

ESMValTool:

• Since April 2018: Porting into ESMValTool by Valeriu Predoi

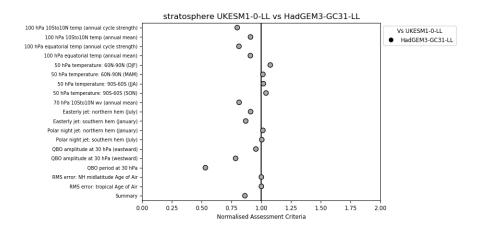


Fig. 55: Standard metrics plot comparing standard metrics from UKESM1-0-LL and HadGEM3-GC31.

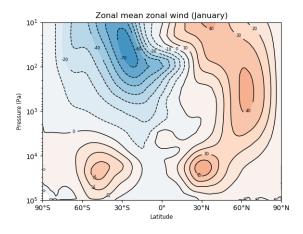


Fig. 56: Zonal mean zonal wind in January for UKESM1-0-LL.

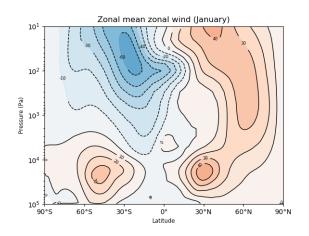


Fig. 57: Zonal mean zonal wind in January for HadGEM3-GC31-LL.

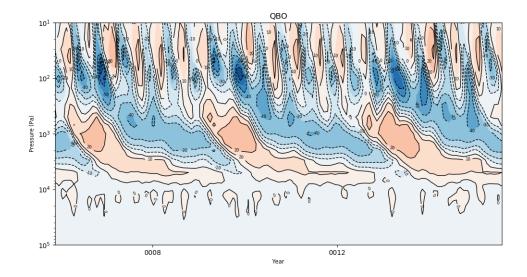


Fig. 58: QBO for UKESM1-0-LL.

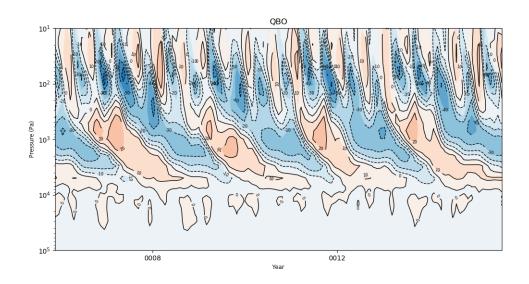


Fig. 59: QBO for HadGEM3-GC31-LL.

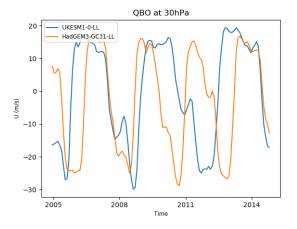


Fig. 60: QBO at 30hPa comparison between UKESM1-0-LL and HadGEM3-GC31-LL.

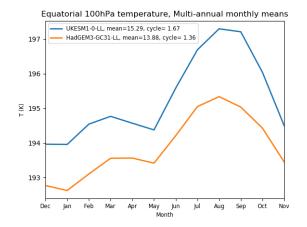


Fig. 61: Equatorial temperature at 100hPa, multi annual means.

#### 15.24.9 Developers

Met Office:

- Prior to May 2008: Neal Butchart
- May 2008 May 2016: Steven C Hardiman

ESMValTool:

• Since April 2018: Valeriu Predoi

# 15.25 Land-surface Permafrost - Autoassess diagnostics

#### 15.25.1 Overview

Permafrost thaw is an important impact of climate change, and is the source of a potentially strong Earth system feedback through the release of soil carbon into the atmosphere. This recipe provides metrics that evaluate the climatological performance of models in simulating soil temperatures that control permafrost. Performance metrics (with observation-based estimates in brackets):

- permafrost area (17.46 million square km)
- fractional area of permafrost northwards of zero degree isotherm (0.47)
- soil temperature at 1m minus soil temperature at surface (-0.53 degrees C)
- soil temperature at surface minus air temperature (6.15 degrees C)
- annual amplitude at 1m / annual amplitude at the surface (0.40 unitless)
- annual amplitude at the surface / annual air temperature (0.57 unitless)

#### Plots:

- · Maps of permafrost extent and zero degC isotherm
- Normalised assessment metrics plot comparing control and experiment

The recipe takes as input a control model and experimental model, comparisons being made with these two models.

#### 15.25.2 Available recipes and diagnostics

Recipes are stored in esmvaltool/recipes/

• recipe\_autoassess\_landsurface\_permafrost.yml

Diagnostics are stored in esmvaltool/diag\_scripts/autoassess/

- autoassess\_area\_base.py: wrapper for autoassess scripts
- land\_surface\_permafrost/permafrost.py: script to calculate permafrost metrics
- plot\_autoassess\_metrics.py: plot normalised assessment metrics

#### 15.25.3 User settings in recipe

1. Script autoassess\_area\_base.py

Required settings for script

- area: must equal land\_surface\_permafrost to select this diagnostic
- control\_model: name of model to be used as control
- exp\_model: name of model to be used as experiment
- start: date (YYYY/MM/DD) at which period begins (see note on time gating)
- end: date (YYYY/MM/DD) at which period ends (see note on time gating)

Optional settings for script

- title: arbitrary string with name of diagnostic
- obs\_models: unused for this recipe

Required settings for variables

none

Optional settings for variables

none

2. Script plot\_autoassess\_metrics.py

Required settings for script

- area: must equal land\_surface\_permafrost to select this diagnostic
- control\_model: name of model to be used as control in metrics plot
- exp\_model: name of model to be used as experiment in metrics plot
- title: string to use as plot title

Optional settings for script

none

Required settings for variables none Optional settings for variables

none

#### 15.25.4 Variables

- tas (atmos, monthly mean, longitude latitude time)
- tsl (land, monthly mean, longitude latitude time)
- mrsos (land, monthly mean, longitude latitude time)
- sftlf (mask, fixed, longitude latitude)

#### 15.25.5 Observations and reformat scripts

None

#### 15.25.6 References

- Observed permafrost extent is from http://nsidc.org/data/ggd318.html: Brown, J., O. Ferrians, J. A. Heginbottom, and E. Melnikov. 2002. Circum-Arctic Map of Permafrost and Ground-Ice Conditions, Version 2. Boulder, Colorado USA. NSIDC: National Snow and Ice Data Center. When calculating the global area of permafrost the grid cells are weighted by the proportion of permafrost within them.
- Annual mean air temperature is from: Legates, D. R., and C. J. Willmott, 1990: Mean seasonal and spatial variability in global surface air temperature. Theor. Appl. Climatol., 41, 11-21. The annual mean is calculated from the seasonal mean data available at the Met Office.
- The soil temperature metrics are calcuated following: Charles D. Koven, William J. Riley, and Alex Stern, 2013: Analysis of Permafrost Thermal Dynamics and Response to Climate Change in the CMIP5 Earth System Models. J. Climate, 26. (Table 3) http://dx.doi.org/10.1175/JCLI-D-12-00228.1 The locations used for Table 3 were extracted from the model and the modelled metrics calculated.

#### 15.25.7 Example plots

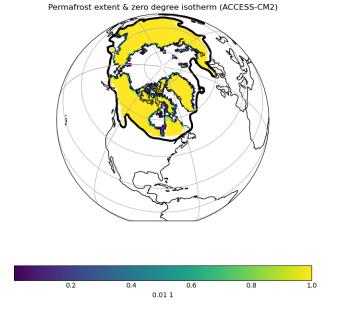


Fig. 62: Permafrost extent and zero degC isotherm, showing North America

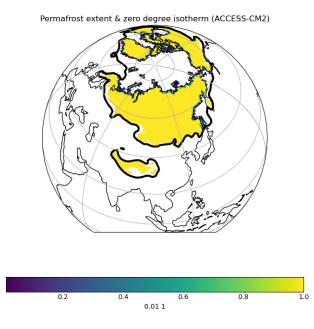


Fig. 63: Permafrost extent and zero degC isotherm, showing Asia and Europe

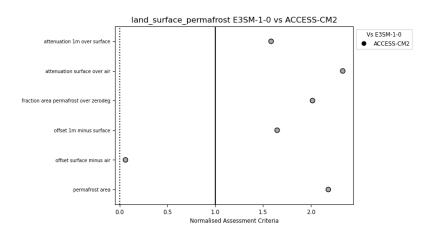


Fig. 64: Normalised metrics plot comparing a control and experiment simulation

#### 15.25.8 Additional notes on usage

The landsurface\_permafrost area metric is part of the esmvaltool/diag\_scripts/autoassess diagnostics, and, as any other autoassess metric, it uses the autoassess\_area\_base.py as general purpose wrapper. This wrapper accepts a number of input arguments that are read through from the recipe.

This recipe is part of the larger group of Autoassess metrics ported to ESMValTool from the native Autoassess package from the UK's Met Office. The diagnostics settings are almost the same as for the other Autoassess metrics.

#### Note: Time gating for autoassess metrics.

To preserve the native Autoassess functionalities, data loading and selection on time is done somewhat differently for ESMValTool's autoassess metrics: the time selection is done in the preprocessor as per usual but a further time selection is performed as part of the diagnostic. For this purpose the user will specify a start: and end: pair of arguments of scripts: autoassess\_script (see below for example). These are formatted as YYYY/MM/DD; this is necessary since the Autoassess metrics are computed from 1-Dec through 1-Dec rather than 1-Jan through 1-Jan. This is a temporary implementation to fully replicate the native Autoassess functionality and a minor user inconvenience since they need to set an extra set of start and end arguments in the diagnostic; this will be phased when all the native Autoassess metrics have been ported to ESMValTool review has completed.

An example of standard inputs as read by autoassess\_area\_base.py and passed over to the diagnostic/metric is listed below.

```
scripts:
plot_landsurf_permafrost: &plot_landsurf_permafrost_settings
        <<: *autoassess_landsurf_permafrost_settings
        control_model: MPI-ESM-LR
        exp_model: MPI-ESM-MR
        script: autoassess/plot_autoassess_metrics.py
        ancestors: ['*/autoassess_landsurf_permafrost']
        title: "Plot Land-Surface Permafrost Metrics"
        plot_name: "Permafrost_Metrics"
        diag_tag: aa_landsurf_permafrost
        diag_name: autoassess_landsurf_permafrost
```

# 15.26 Land-surface Surface Radiation - Autoassess diagnostics

#### 15.26.1 Overview

The simulation of surface radiation is central to all aspects of model performance, and can often reveal compensating errors which are hidden within top of atmosphere fluxes. This recipe provides metrics that evaluate the skill of models' spatial and seasonal distribution of surface shortwave and longwave radiation against the CERES EBAF satellite dataset.

Performance metrics:

- median absolute error (model minus observations) net surface shortwave (SW) radiation
- median absolute error (model minus observations) net surface longwave (LW) radiation

Metrics are calculated using model and observation multi-year climatologies (seasonal means) for meteorological seasons: \* December-January-February (djf) \* March-April-May (mam) \* June-July-August (jja) \* September-October-November (son) \* Annual mean (ann)

Plots:

• Normalised assessment metrics plot comparing control and experiment

The recipe takes as input a control model and experimental model, comparisons being made with these two models.

#### 15.26.2 Available recipes and diagnostics

Recipes are stored in esmvaltool/recipes/

recipe\_autoassess\_landsurface\_surfrad.yml

Diagnostics are stored in esmvaltool/diag\_scripts/autoassess/

- autoassess\_area\_base.py: wrapper for autoassess scripts
- land\_surface\_surfrad/surfrad.py: script to calculate surface radiation metrics
- plot\_autoassess\_metrics.py: plot normalised assessment metrics

#### 15.26.3 User settings in recipe

1. Script autoassess\_area\_base.py

Required settings for script

- area: must equal land\_surface\_surfrad to select this diagnostic
- control\_model: name of model to be used as control
- exp\_model: name of model to be used as experiment
- start: date (YYYY/MM/DD) at which period begins (see note on time gating)
- end: date (YYYY/MM/DD) at which period ends (see note on time gating)
- climfiles\_root: path to observation climatologies

#### Optional settings for script

- title: arbitrary string with name of diagnostic
- obs\_models: unused for this recipe

Required settings for variables

#### none

Optional settings for variables

none

2. Script plot\_autoassess\_metrics.py

#### Required settings for script

- area: must equal land\_surface\_surfrad to select this diagnostic
- control\_model: name of model to be used as control in metrics plot
- exp\_model: name of model to be used as experiment in metrics plot
- title: string to use as plot title

```
Optional settings for script
none
Required settings for variables
none
Optional settings for variables
none
```

#### 15.26.4 Variables

- rsns (atmos, monthly mean, longitude latitude time)
- rlns (atmos, monthly mean, longitude latitude time)
- sftlf (mask, fixed, longitude latitude)

#### 15.26.5 Observations and reformat scripts

2001-2012 climatologies (seasonal means) from CERES-EBAF Ed2.7.

#### 15.26.6 References

- Loeb, N. G., D. R. Doelling, H. Wang, W. Su, C. Nguyen, J. G. Corbett, L. Liang, C. Mitrescu, F. G. Rose, and S. Kato, 2018: Clouds and the Earth's Radiant Energy System (CERES) Energy Balanced and Filled (EBAF) Top-of-Atmosphere (TOA) Edition-4.0 Data Product. J. Climate, 31, 895-918, doi: 10.1175/JCLI-D-17-0208.1.
- Kato, S., F. G. Rose, D. A. Rutan, T. E. Thorsen, N. G. Loeb, D. R. Doelling, X. Huang, W. L. Smith, W. Su, and S.-H. Ham, 2018: Surface irradiances of Edition 4.0 Clouds and the Earth's Radiant Energy System (CERES) Energy Balanced and Filled (EBAF) data product, J. Climate, 31, 4501-4527, doi: 10.1175/JCLI-D-17-0523.1

#### 15.26.7 Example plots

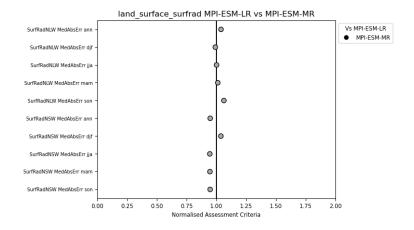


Fig. 65: Normalised metrics plot comparing a control and experiment simulation

#### 15.26.8 Inputs and usage

The landsurface\_soilmoisture area metric is part of the esmvaltool/diag\_scripts/autoassess diagnostics, and, as any other autoassess metric, it uses the autoassess\_area\_base.py as general purpose wrapper. This wrapper accepts a number of input arguments that are read through from the recipe.

This recipe is part of the larger group of Autoassess metrics ported to ESMValTool from the native Autoassess package from the UK's Met Office. The diagnostics settings are almost the same as for the other Autoassess metrics.

#### Note: Time gating for autoassess metrics.

To preserve the native Autoassess functionalities, data loading and selection on time is done somewhat differently for ESMValTool's autoassess metrics: the time selection is done in the preprocessor as per usual but a further time selection is performed as part of the diagnostic. For this purpose the user will specify a start: and end: pair of arguments of scripts: autoassess\_script (see below for example). These are formatted as YYYY/MM/DD; this is necessary since the Autoassess metrics are computed from 1-Dec through 1-Dec rather than 1-Jan through 1-Jan. This is a temporary implementation to fully replicate the native Autoassess functionality and a minor user inconvenience since they need to set an extra set of start and end arguments in the diagnostic; this will be phased when all the native Autoassess metrics have been ported to ESMValTool review has completed.

An example of standard inputs as read by autoassess\_area\_base.py and passed over to the diagnostic/metric is listed below.

```
scripts:
autoassess_landsurf_surfrad: &autoassess_landsurf_surfrad_settings
script: autoassess/autoassess_area_base.py
title: "Autoassess Land-Surface Diagnostic Surfrad Metric"
area: land_surface_surfrad
control_model: UKESM1-0-LL
exp_model: UKESM1-0-LL
obs_models: [CERES-EBAF]
obs_type: obs4MIPs
start: 1997/12/01
end: 2002/12/01
```

# 15.27 Land-surface Soil Moisture - Autoassess diagnostics

#### 15.27.1 Overview

Soil moisture is a critical component of the land system, controling surface energy fluxes in many areas of the world. This recipe provides metrics that evaluate the skill of models' spatial and seasonal distribution of soil moisture against the ESA CCI soil moisture ECV.

Performance metrics:

• median absolute error (model minus observations)

Metrics are calculated using model and observation multi-year climatologies (seasonal means) for meteorological seasons:

- December-January-February (djf)
- March-April-May (mam)
- June-July-August (jja)

• September-October-November (son)

Plots:

· Normalised assessment metrics plot comparing control and experiment

The recipe takes as input a control model and experimental model, comparisons being made with these two models.

#### 15.27.2 Available recipes and diagnostics

Recipes are stored in esmvaltool/recipes/

· recipe\_autoassess\_landsurface\_soilmoisture.yml

Diagnostics are stored in esmvaltool/diag\_scripts/autoassess/

- land\_surface\_soilmoisture/soilmoisture.py: script to calculate soil moisture metrics
- plot\_autoassess\_metrics.py: plot normalised assessment metrics

#### 15.27.3 User settings in recipe

1. Script soilmoisture.py

Required settings for script

- area: must equal land\_surface\_soilmoisture to select this diagnostic
- control\_model: name of model to be used as control
- exp\_model: name of model to be used as experiment

Optional settings for script

none

Required settings for variables

none

Optional settings for variables

none

2. Script plot\_autoassess\_metrics.py

Required settings for script

- area: must equal land\_surface\_soilmoisture to select this diagnostic
- control\_model: name of model to be used as control in metrics plot
- exp\_model: name of model to be used as experiment in metrics plot
- title: string to use as plot title

Optional settings for script

none

```
Required settings for variables
none
Optional settings for variables
none
```

#### 15.27.4 Variables

- mrsos (from models: land, monthly mean, longitude latitude time)
- sm (from observations: land, monthly mean, longitude latitude time)

## 15.27.5 Observations and reformat scripts

1999-2008 climatologies (seasonal means) from ESA ECV Soil Moisture Dataset v1. Produced by the ESA CCI soil moisture project: https://www.esa-soilmoisture-cci.org/node/93

## 15.27.6 References

- Dorigo, W.A., Wagner, W., Albergel, C., Albrecht, F., Balsamo, G., Brocca, L., Chung, D., Ertl, M., Forkel, M., Gruber, A., Haas, E., Hamer, D. P. Hirschi, M., Ikonen, J., De Jeu, R. Kidd, R. Lahoz, W., Liu, Y.Y., Miralles, D., Lecomte, P. (2017). ESA CCI Soil Moisture for improved Earth system understanding: State-of-the art and future directions. In Remote Sensing of Environment, 2017, ISSN 0034-4257, https://doi.org/10.1016/j.rse.2017.07. 001.
- Gruber, A., Scanlon, T., van der Schalie, R., Wagner, W., Dorigo, W. (2019). Evolution of the ESA CCI Soil Moisture Climate Data Records and their underlying merging methodology. Earth System Science Data 11, 717-739, https://doi.org/10.5194/essd-11-717-2019

## 15.27.7 Example plots

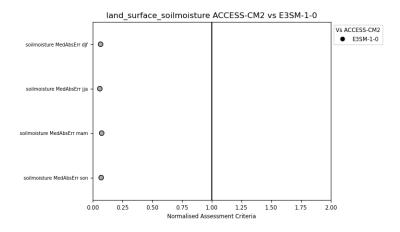


Fig. 66: Normalised metrics plot comparing a control and experiment simulation

# 15.28 Stratosphere-troposphere coupling and annular modes indices (ZMNAM)

#### 15.28.1 Overview

The current generation of climate models include the representation of stratospheric processes, as the vertical coupling with the troposphere is important for the weather and climate at the surface (e.g., Baldwin and Dunkerton, 2001).

The recipe recipe\_zmnam.yml can be used to evaluate the representation of Annular Modes (AM, e.g., Wallace, 2000) in climate simulations, using reanalysis datasets as reference.

The calculation is based on the "zonal mean algorithm" of Baldwin and Thompson (2009), and is alternative to pressure based or height-dependent methods.

This approach provides a robust description of the stratosphere-troposphere coupling on daily timescales, requiring less subjective choices and a reduced amount of input data. Starting from daily mean geopotential height on pressure levels, the leading empirical orthogonal function/principal component are computed from zonal mean daily anomalies, with the leading principal component representing the zonal mean AM index. The regression of the monthly mean geopotential height onto this monthly averaged index represents the AM pattern for each selected pressure level.

The outputs of the procedure are the monthly time series and the histogram of the daily zonal mean AM index, and the monthly regression maps for selected pressure levels. The users can select the specific datasets (climate model simulation and/or reanalysis) to be evaluated, the Northern or Southern hemisphere (NH or SH) and a subset of pressure levels of interest.

## 15.28.2 Available recipes and diagnostics

Recipes are stored in recipes/

• recipe\_zmnam.yml

Diagnostics are stored in diag\_scripts/zmnam/

• zmnam.py

and subroutines

- zmnam\_calc.py
- zmnam\_plot.py
- zmnam\_preproc.py

#### 15.28.3 User settings

Hemisphere of interest (NH or SH)

#### 15.28.4 Variables

• zg (atmos, daily mean, longitude latitude time)

## 15.28.5 Observations and reformat scripts

None.

#### 15.28.6 References

- Baldwin, M. P. and Thompson, D. W. (2009), A critical comparison of stratosphere–troposphere coupling indices. Q.J.R. Meteorol. Soc., 135: 1661-1672. doi:10.1002/qj.479.
- Baldwin, M. P and Dunkerton, T. J. (2001), Stratospheric Harbingers of Anomalous Weather Regimes. Science 294 (5542): 581-584. doi:10.1126/science.1063315.
- Wallace, J. M. (2000), North Atlantic Oscillation/annular mode: Two paradigms-one phenomenon. Q.J.R. Meteorol. Soc., 126 (564): 791-805. doi:10.1002/qj.49712656402.

## 15.28.7 Example plots

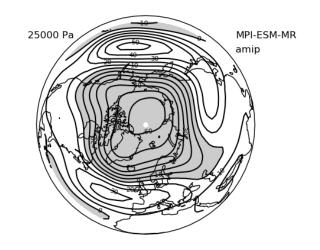


Fig. 67: Regression map of the Northern Hemisphere zonal mean AM index onto geopotential height, for a selected pressure level (250 hPa) for the MPI-ESM-MR model (CMIP5 AMIP experiment, period 1979-2008). Negative values are shaded in grey.

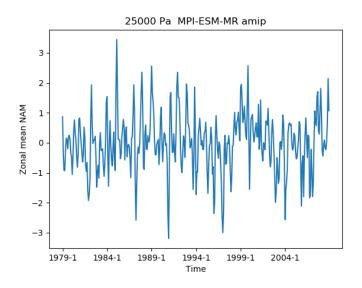


Fig. 68: Time series of the Northern Hemisphere zonal mean AM index for a selected pressure level (250 hPa) for the MPI-ESM-MR model (CMIP5 AMIP experiment, period 1979-2008).

# 15.29 Thermodynamics of the Climate System - The Diagnostic Tool TheDiaTo v1.0

#### 15.29.1 Overview

The tool allows to compute TOA, atmospheric and surface energy budgets, latent energy and water mass budgets, meridional heat transports, the Lorenz Energy Cycle (LEC), the material entropy production with the direct and indirect method.

The energy budgets are computed from monthly mean radiative and heat fluxes at the TOA and at the surface (cfr. Wild et al., 2013). The meridional heat transports are obtained from the latitudinal integration of the zonal mean energy budgets. When a land-sea mask is provided, results are also available for land and oceans, separately.

The water mass budget is obtained from monthly mean latent heat fluxes (for evaporation), total and snowfall precipitation (cfr. Liepert et al., 2012). The latent energy budget is obtained multiplying each component of the water mass budget by the respective latent heat constant. When a land-sea mask is provided, results are also available for land and oceans, separately.

The LEC is computed from 3D fields of daily mean velocity and temperature fields in the troposphere over pressure levels. The analysis is carried on in spectral fields, converting lonlat grids in Fourier coefficients. The components of the LEC are computed as in Ulbrich and Speth, 1991. In order to account for possible gaps in pressure levels, the daily fields of 2D near-surface temperature and horizontal velocities are needed. These are required to perform a vertical interpolation, substituting data in pressure levels where surface pressure is lower than the respective level and fields are not stored as an output of the analysed model.

The material entropy production is computed by using the indirect or the direct method (or both). The former method relies on the convergence of radiative heat in the atmosphere (cfr. Lucarini et al., 2011; Pascale et al., 2011), the latter on all viscous and non-viscous dissipative processes occurring in the atmosphere (namely the sensible heat fluxes, the hydrological cycle with its components and the kinetic energy dissipation).

For a comprehensive report on the methods used and some descriptive results, please refer to Lembo et al., 2019.

In order to account for possible gaps in pressure levels, the daily fields of 2D near-surface temperature and horizontal

velocities.'

#### 15.29.2 Available recipes and diagnostics

Recipes are stored in recipes/

• recipe\_thermodyn\_diagtool.yml

Diagnostics are stored in diag\_scripts/thermodyn\_diagtool/

- thermodyn\_diagnostics.py: the main script, handling input files, calling computation and plotting scricpts;
- computations.py: a module containing all the main computations that are carried out by the program;
- fluxogram.py: a module for the retrieval of the block diagrams displaying the reservoirs and conversion terms of the LEC
- fourier\_coefficients.py: a module for the computation of the Fourier coefficients from the lonlat input grid
- lorenz\_cycle.py: a module for the computation of the LEC components in Fourier coefficients
- mkthe.py: a module for the computation of indirect variables obtained from the input fields, such as LCL height, boundary layer top height and temperature, potential temperature
- plot\_script.py: a module for the computation of maps, scatter plots, time series and meridional sections of some derived quantities for each model in the ensemble. The meridional heat and water mass transports are also computed here, as well as the peak magnitudes and locations;
- provenance\_meta.py: a module for collecting metadata and writing them to produced outputs;

#### 15.29.3 User settings

Besides the datasets, to be set according to usual ESMValTool convention, the user can set the following optional variables in the recipe\_Thermodyn\_diagtool.yml:

- wat: if set to 'true', computations are performed of the water mass and latent energy budgets and transports
- lsm: if set to true, the computations of the energy budgets, meridional energy transports, water mass and latent energy budgets and transports are performed separately over land and oceans
- lec: if set to 'true', computation of the LEC are performed
- entr: if set to 'true', computations of the material entropy production are performed
- met (1, 2 or 3): the computation of the material entropy production must be performed with the indirect method (1), the direct method (2), or both methods. If 2 or 3 options are chosen, the intensity of the LEC is needed for the entropy production related to the kinetic energy dissipation. If lec is set to 'false', a default value is provided.

These options apply to all models provided for the multi-model ensemble computations

#### 15.29.4 Variables

Default variables needed for computation of energy budgets and transports:

- hfls (atmos, monthly mean, time latitude longitude)
- hfss (atmos, monthly mean, time latitude longitude)
- rlds (atmos, monthly mean, time latitude longitude)
- rlus (atmos, monthly mean, time latitude longitude)
- rlut (atmos, monthly mean, time latitude longitude)
- rsds (atmos, monthly mean, time latitude longitude)
- rsdt (atmos, monthly mean, time latitude longitude)
- rsus (atmos, monthly mean, time latitude longitude)
- rsut (atmos, monthly mean, time latitude longitude)

Additional variables needed for water mass and latent energy computation (optional, with 'wat' set to 'true'):

- pr (atmos, monthly mean, time latitude longitude)
- prsn (atmos, monthly mean, time latitude longitude)

Additional variable needed for LEC computations (optional, with 'lec' set to 'true'):

- ta (atmos, daily mean, time plev latitude longitude)
- tas (atmos, daily mean, time latitude longitude)
- ua (atmos, daily mean, time plev latitude longitude)
- uas (atmos, daily mean, time latitude longitude)
- va (atmos, daily mean, time plev latitude longitude)
- vas (atmos, daily mean, time latitude longitude)
- wap (atmos, daily mean, time plev latitude longitude)

Additional variables needed for material entropy production computations with direct method (optional, with 'entr' set to 'true' and 'mep' to '2' or '3'):

- hus (atmos, monthly mean, time plev latitude longitude)
- pr (atmos, monthly mean, time latitude longitude)
- prsn (atmos, monthly mean, time latitude longitude)
- ps (atmos, monthly mean, time latitude longitude)
- ts (atmos, monthly mean, time latitude longitude)

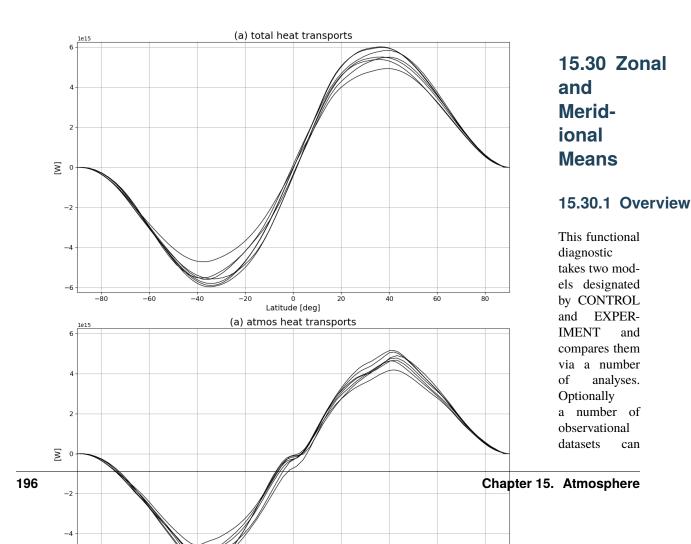
Additional variables needed for material entropy production computations with indirect method (optional, with 'entr' set to 'true' and 'mep' to '1' or '3'):

- tas (atmos, daily mean, time latitude longitude)
- uas (atmos, daily mean, time latitude longitude)
- vas (atmos, daily mean, time latitude longitude)

Depending on the user's options, variables listed above must be provided. All other variables shall be commented in the recipe file.

#### 15.29.5 References

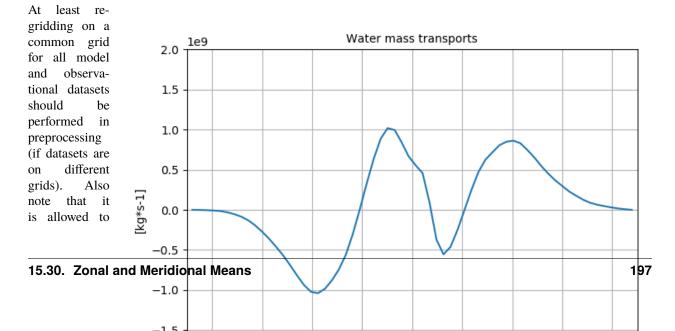
- Lembo V, Lunkeit F, Lucarini V (2019) A new diagnostic tool for diagnosing water, energy and entropy budgets in climate models. Geophys Mod Dev Disc. doi:10.5194/gmd-12-3805-2019
- Liepert BG, Previdi M (2012) Inter-model variability and biases of the global water cycle in CMIP3 coupled climate models. Environ Res Lett 7:014006. doi: 10.1088/1748-9326/7/1/014006
- Lorenz EN (1955) Available Potential Energy and the Maintenance of the General Circulation. Tellus 7:157–167. doi: 10.1111/j.2153-3490.1955.tb01148.x
- Lucarini V, Fraedrich K, Ragone F (2010) New Results on the Thermodynamical Properties of the Climate System. J Atmo 68:. doi: 10.1175/2011JAS3713.1
- Lucarini V, Blender R, Herbert C, et al (2014) Reviews of Geophysics Mathematical and physical ideas for climate science. doi: 10.1002/2013RG000446
- Pascale S, Gregory JM, Ambaum M, Tailleux R (2011) Climate entropy budget of the HadCM3 atmosphere–ocean general circulation model and of FAMOUS, its low-resolution version. Clim Dyn 36:1189–1206. doi: 10.1007/s00382-009-0718-1
- Ulbrich U, Speth P (1991) The global energy cycle of stationary and transient atmospheric waves: Results from ECMWF analyses. Meteorol Atmos Phys 45:125–138. doi: 10.1007/BF01029650
- Wild M, Folini D, Schär C, et al (2013) The global energy balance from a surface perspective. Clim Dyn 40:3107–3134. doi: 10.1007/s00382-012-1569-8



#### 15.29.6 Example plots

be added for processing. There are three types of standard analysis: lat lon, meridional mean and zonal mean. Each of these diagnostics can be run on a separate basis (each an entry diagnosto tics/scripts). The lat\_lon analysis produces the following plots: a simple global plot for each variable for each dataset, a global plot for the difference between CONTROL EXPERand IMENT, а global plot for the difference between CON-TROL and

each of the observational datasets. The meridional\_mean and zonal\_mean produce variable vs coordinate (latitude or longitude) with both CONTROL and EXPERIMENT curves in each plot, for the entire duration of time specified and also, if the user wishes, for each season (seasonal means): winter DJF, spring MAM, summer JJA, autumn SON (by setting seasonal\_analysis: true in the recipe).



use the same dataset (with varying parameters like experiment or ensemble or mip) for both CONTROL and EXPER-IMENT (as long as at least one data parameter is different).

## 15.30.2 Available recipes and diagnostics

Recipes are stored in recipes/

- recipe\_validation.yml (CMIP5)
- recipe\_validation\_CMIP6.yml (CMIP6)

Diagnostics are stored in diag\_scripts/

- validation.py
- shared/\_validation.py

#### 15.30.3 User settings

1. validation.py

Required settings for script

- title: title of the analysis, user defined;
- control\_model: control dataset name e.g. UKESM1-0-LL;
- exper\_model: experiment dataset name e.g. IPSL-CM6A-LR;
- observational\_datasets: list of at least one element; if no OBS wanted comment out; e.g. ['ERA-Interim'];
- analysis\_type: use any of: lat\_lon, meridional\_mean, zonal\_mean;
- seasonal\_analysis: boolean, if seasonal means are needed e.g. true;
- save\_cubes: boolean, save each of the plotted cubes in /work;

#### 15.30.4 Variables

• any variable

## 15.30.5 Observations and reformat scripts

Note: (1) obs4MIPs or OBS or ana4mips can be used.

- · any observations
- it is important to note that all observational data should go through the same preprocessing as model data

## 15.30.6 References

• none, basic technical analysis

## 15.30.7 Example plots

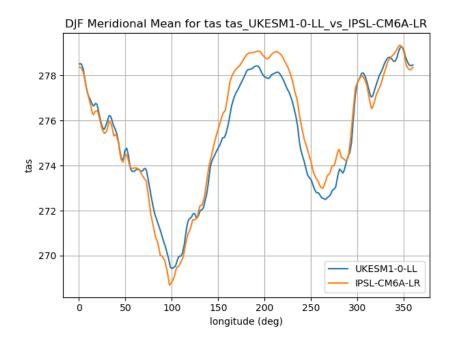


Fig. 69: Meridional seasonal mean for winter (DJF) comparison beween CMIP6 UKESM1 and IPSL models.

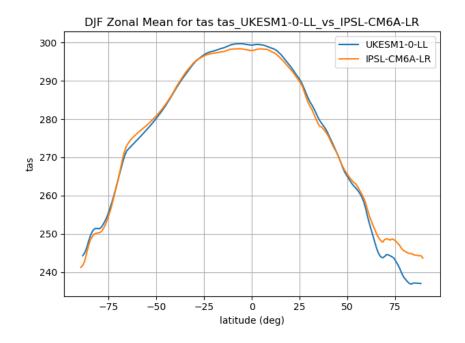


Fig. 70: Zonal seasonal mean for winter (DJF) comparison beween CMIP6 UKESM1 and IPSL models.

# 15.31 Radiation Budget

## 15.31.1 Overview

The aim of monitoring the energy budget is to understand the (im)balance of energy flux between the atmosphere and the surface of a model due to its link with the hydrological cycle and climate change.

This diagnostic analyses the radiation budget by separating top-of-atmosphere fluxes into clear-sky and cloud forcing components, and surface fluxes into downwelling and upwelling components. Model predictions are compared against three observational estimates, one of which (Stephens et al. 2012) includes uncertainty estimates. When the black error bars overlap the zero line, the model is consistent with observations according to Stephens et al. (2012).

## 15.31.2 Available recipes and diagnostics

Recipes are stored in esmvaltool/recipes/

recipe\_radiation\_budget.yml

Diagnostics are stored in esmvaltool/diag\_scripts/radiation\_budget/

- radiation\_budget.py: Plot the global radiation budget.
- seasonal\_radiation\_budget.py: Write the global climatological seasonal radiation budget to a text file.

#### 15.31.3 User settings in recipe

None

#### 15.31.4 Variables

- rss (atmos, monthly mean, longitude latitude time)
- rsdt (atmos, monthly mean, longitude latitude time)
- rsut (atmos, monthly mean, longitude latitude time)
- rsutcs (atmos, monthly mean, longitude latitude time)
- rsds (atmos, monthly mean, longitude latitude time)
- rls (atmos, monthly mean, longitude latitude time)
- rlut (atmos, monthly mean, longitude latitude time)
- rlutcs (atmos, monthly mean, longitude latitude time)
- rlds (atmos, monthly mean, longitude latitude time)
- hfss (atmos, monthly mean, longitude latitude time)
- hfls (atmos, monthly mean, longitude latitude time)

## 15.31.5 Observations and reformat scripts

Note: (1) obs4MIPs data can be used directly without any preprocessing; (2) see headers of reformat scripts for nonobs4MIPs data for download instructions.

- CERES-EBAF (rlut, rlutcs, rsut, rsutcs obs4MIPs)
- Demory observations can be found in esmvaltool/diag\_scripts/radiation\_budget/Demory\_et\_al\_2014\_obs\_Energy\_Budget.yml and are from Figure 2 in Demory et al. (2014).
- Stephens observations can be found in esmvaltool/diag\_scripts/radiation\_budget/Stephens\_et\_al\_2012\_obs\_Energy\_Budget.yml from figure 1b in Stephens et al. (2012).

#### 15.31.6 References

- Demory, ME., Vidale, P.L., Roberts, M.J. et al. The role of horizontal resolution in simulating drivers of the global hydrological cycle. Clim Dyn 42, 2201–2225 (2014). https://doi.org/10.1007/s00382-013-1924-4
- Stephens, G., Li, J., Wild, M. et al. An update on Earth's energy balance in light of the latest global observations. Nature Geosci 5, 691–696 (2012). https://doi.org/10.1038/ngeo1580

#### 15.31.7 Example plots

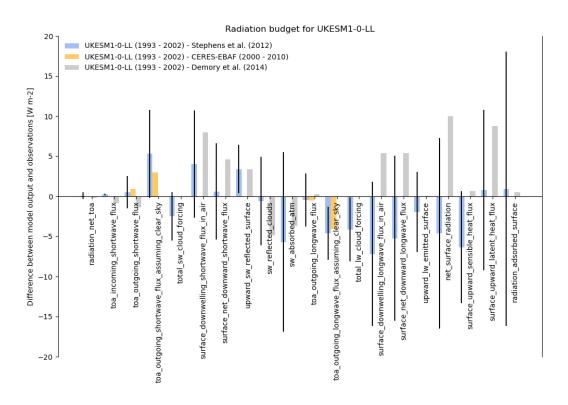


Fig. 71: Radiation budget for UKESM1-0-LL

# 15.32 AOD AeroNET Assess

#### 15.32.1 Overview

This diagnostic evaluates model aerosol optical depth (AOD) against ground based observations from the AeroNET measurement network. Monthly mean AOD data is downloaded from the AeroNET website and formatted (CMORized) using the AERONET downloader and formatter within ESMValTool.

Multiannual seasonal means are calculated from the model output and compared with a multiannual seasonal mean climatology generated from AeroNET observational data. At each AeroNET station the data are screened for validity according to the following default criteria:

- 1. Monthly means must be generated from at least one AOD observation in that month.
- 2. Seasonal means for DJF, MAM, JJA and SON must be calculated from three monthly means, i.e. a monthly mean from December January and Feburary.
- 3. For a given year to be valid, there must be a seasonal mean for each climate season i.e. DJF, MAM, JJA and SON.
- 4. For a multiannual seasonal means there must be at least five seasonaal means over the time range of interest.

NOTE: The code is designed to be flexible and the default criteria can be changed according to the user's requirements (see the user settings below).

The evaluation is visualised by plotting model output as 2D filled contours and overlaying AeroNET observations at model grid cells co-located with the AeroNET measurement stations. Statistical data (root mean square error) is generated using AeroNET observations at model grid cells co-located with the AeroNET measurement stations.

#### 15.32.2 Available recipes and diagnostics

Recipes are stored in esmvaltool/recipes/

recipe\_aod\_aeronet\_assess.yml

Diagnostics are stored in esmvaltool/diag\_scripts/aerosols/

- aod\_aeronet\_assess.py: Plot the AOD evaluation.
- aero\_utils.py: Utility functions commonly used by aerosol assessment routines.

#### 15.32.3 User settings in recipe

1. Script aod\_aeronet\_assess.py

Required settings for script

- wavel: The wavelength of interest for the evaluation, currently set up for 440nm
- min\_days\_per\_mon: The minimum number of days used to calculate the AOD monthly mean
- min\_mon\_per\_seas: The minimum number of seasons used to calculate each seasonal mean. This must be between 1 and 3.
- min\_seas\_per\_year: The minimum number of seasonal means in each year. This must be between 1 and 4.
- min\_seas\_per\_clim: The minimum number of seasonal means used to calculate the multiannual seasonal mean. This must be between 1 and the number of years of available AeroNET data.

Optional settings for script

• None

Required settings for variables

• None

*Optional settings for variables* 

• None

Required settings for preprocessor

• None

Optional settings for preprocessor

• None

Color tables

• brewer\_Spectral\_11

#### 15.32.4 Variables

• od440aer (atmos, monthly mean, longitude latitude time)

#### 15.32.5 Observations and reformat scripts

- Note: (1) obs4MIPs data can be used directly without any preprocessing; (2) see headers of reformat scripts for non-obs4MIPs data for download instructions.
- The AeroNET data is downloaded from the AeroNET website using the downloader:

```
$ esmvaltool data download AERONET.
```

• The AeroNET data is formatteed (CMORized) using the formatter:

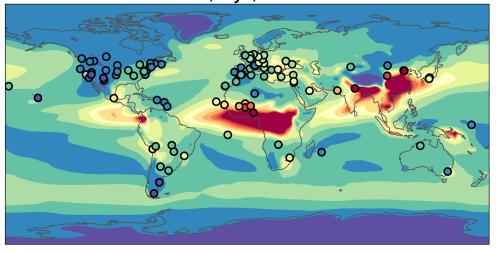
```
$ esmvaltool data format AERONET.
```

#### 15.32.6 References

- Holben B.N., T.F.Eck, I.Slutsker, D.Tanre, J.P.Buis, A.Setzer, E.Vermote, J.A.Reagan, Y.Kaufman, T.Nakajima, F.Lavenu, I.Jankowiak, and A.Smirnov, 1998: AERONET - A federated instrument network and data archive for aerosol characterization, Rem. Sens. Environ., 66, 1-16.
- Holben, B.N., D.Tanre, A.Smirnov, T.F.Eck, I.Slutsker, N.Abuhassan, W.W.Newcomb, J.Schafer, B.Chatenet, F.Lavenue, Y.J.Kaufman, J.Vande Castle, A.Setzer, B.Markham, D.Clark, R.Frouin, R.Halthore, A.Karnieli, N.T.O'Neill, C.Pietras, R.T.Pinker, K.Voss, and G.Zibordi, 2001: An emerging ground-based aerosol climatology: Aerosol Optical Depth from AERONET, J. Geophys. Res., 106, 12 067-12 097.
- Mulcahy, J. P., Johnson, C., Jones, C. G., Povey, A. C., Scott, C. E., Sellar, A., Turnock, S. T., Woodhouse, M. T., Abraham, N. L., Andrews, M. B., Bellouin, N., Browse, J., Carslaw, K. S., Dalvi, M., Folberth, G. A., Glover, M., Grosvenor, D. P., Hardacre, C., Hill, R., Johnson, B., Jones, A., Kipling, Z., Mann, G., Mollard, J., O'Connor, F. M., Palmiéri, J., Reddington, C., Rumbold, S. T., Richardson, M., Schitgens, N. A. J., Stier, P., Stringer, M., Tang, Y., Walton, J., Woodward, S., and Yool. A.: Description and evaluation of aerosol in UKESM1 and HadGEM3-GC3.1 CMIP6 historical simulations, Geosci. Model Dev., 13, 6383–6423, 2020

#### 15.32.7 Example plots

# Total Aerosol Optical Depth at 0.44 microns UKESM1-0-LL, DJF, N stations=107

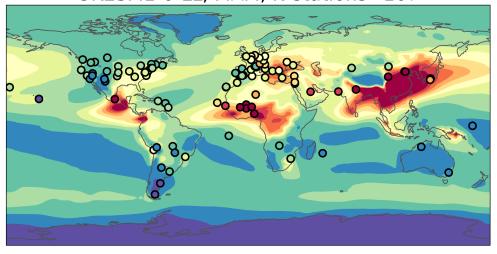


Global mean AOD= 0.160; RMSE= 0.082; Stn mean: md= 0.161; obs= 0.171



Fig. 72: Evaluation of AOD at 440 nm from UKESM1 historical ensemble member r1i1p1f2 against the AeroNET climatology from ground-based observations for Dec-Jan-Feb. The multiannual seasonal mean is calculated for the model data for the period 1994-2014. The model output is overlaid with the observational climatology.

## Total Aerosol Optical Depth at 0.44 microns UKESM1-0-LL, MAM, N stations=107

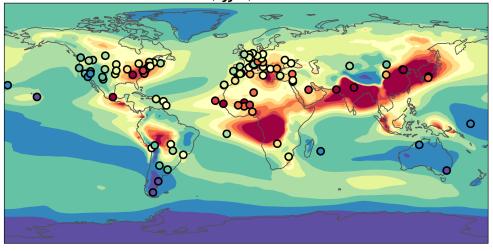


Global mean AOD= 0.177; RMSE= 0.105; Stn mean: md= 0.234; obs= 0.244



Fig. 73: Evaluation of AOD at 440 nm from UKESM1 historical ensemble member r1i1p1f2 against the AeroNET climatology from ground-based observations for Mar\_Apr\_May. The multiannual seasonal mean is calculated for the model data for the period 1994-2014. The model output is overlaid with the observational climatology.

# Total Aerosol Optical Depth at 0.44 microns UKESM1-0-LL, JJA, N stations=107



Global mean AOD= 0.194; RMSE= 0.121; Stn mean: md= 0.290; obs= 0.285

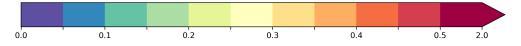
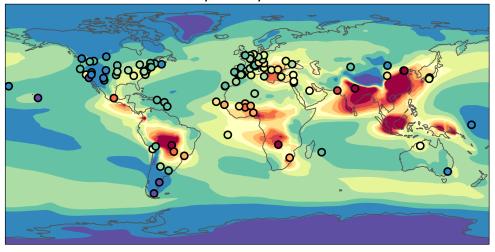


Fig. 74: Evaluation of AOD at 440 nm from UKESM1 historical ensemble member r1i1p1f2 against the AeroNET climatology from ground-based observations for Jun-Jul-Aug. The multiannual seasonal mean is calculated for the model data for the period 1994-2014. The model output is overlaid with the observational climatology.

# Total Aerosol Optical Depth at 0.44 microns UKESM1-0-LL, SON, N stations=107



Global mean AOD= 0.178; RMSE= 0.089; Stn mean: md= 0.213; obs= 0.212



Fig. 75: Evaluation of AOD at 440 nm from UKESM1 historical ensemble member r1i1p1f2 against the AeroNET climatology from ground-based observations for Sep-Oct-Nov. The multiannual seasonal mean is calculated for the model data for the period 1994-2014. The model output is overlaid with the observational climatology.

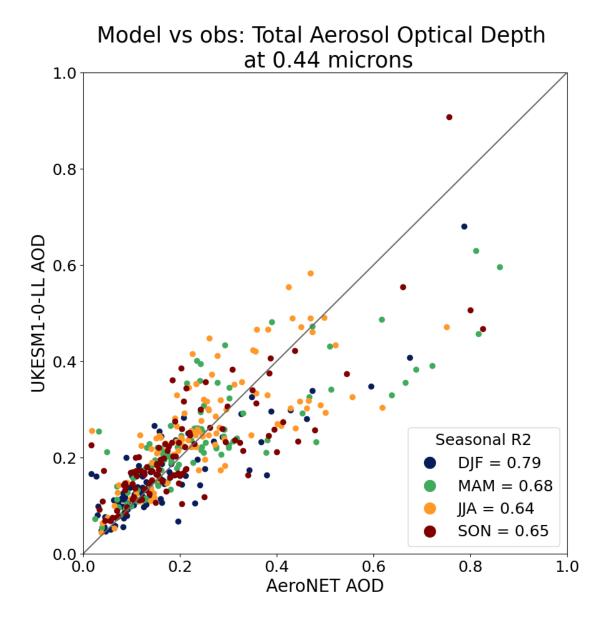


Fig. 76: Evaluation of AOD at 440 nm from UKESM1 historical ensemble member r1i1p1f2 against the AeroNET climatology from ground-based observations for Dec-Jan-Feb, Mar\_Apr\_May, Jun-Jul-Aug and Sep-Oct-Nov. The multiannual seasonal mean is calculated for the model data for the period 1994-2014.

## CHAPTER

# SIXTEEN

# **CLIMATE METRICS**

# **16.1 Performance metrics for essential climate parameters**

## 16.1.1 Overview

The goal is to create a standard recipe for the calculation of performance metrics to quantify the ability of the models to reproduce the climatological mean annual cycle for selected "Essential Climate Variables" (ECVs) plus some additional corresponding diagnostics and plots to better understand and interpret the results.

The recipe can be used to calculate performance metrics at different vertical levels (e.g., 5, 30, 200, 850 hPa as in Gleckler et al. (2008) and in different regions. As an additional reference, we consider Righi et al. (2015).

## 16.1.2 Available recipes and diagnostics

Recipes are stored in recipes/

- recipe\_perfmetrics\_CMIP5.yml
- recipe\_perfmetrics\_CMIP5\_4cds.yml
- recipe\_perfmetrics\_land\_CMIP5.yml

Diagnostics are stored in diag\_scripts/perfmetrics/

- main.ncl: calculates and (optionally) plots annual/seasonal cycles, zonal means, lat-lon fields and time-lat-lon fields. The calculated fields can also be plotted as difference w.r.t. a given reference dataset. main.ncl also calculates RMSD, bias and taylor metrics. Input data have to be regridded to a common grid in the preprocessor. Each plot type is created by a separated routine, as detailed below.
- cycle.ncl: creates an annual/seasonal cycle plot.
- zonal.ncl: creates a zonal (lat-pressure) plot.
- latlon.ncl: creates a lat-lon plot.
- cycle\_latlon.ncl: precalculates the metrics for a time-lat-lon field, with different options for normalization.
- collect.ncl: collects and plots the metrics previously calculated by cycle\_latlon.ncl.

# 16.1.3 User settings in recipe

1. Script main.ncl

Required settings (scripts)

- plot\_type: cycle (time), zonal (plev, lat), latlon (lat, lon), cycle\_latlon (time, lat, lon), cycle\_zonal (time, plev, lat)
- time\_avg: type of time average (monthlyclim, seasonalclim, annualclim)
- region: selected region (global, trop, nhext, shext, nhtrop, shtrop, nh, sh, nhmidlat, shmidlat, nhpolar, shpolar, eq)

Optional settings (scripts)

- styleset: for plot\_type cycle only (cmip5, righi15gmd, cmip6, default)
- plot\_stddev: for plot\_type cycle only, plots standard deviation as shading
- legend\_outside: for plot\_type cycle only, plots the legend in a separate file
- t\_test: for plot\_type zonal or latlon, calculates t-test in difference plots (default: False)
- conf\_level: for plot\_type zonal or latlon, adds the confidence level for the t-test to the plot (default: False)
- projection: map projection for plot\_type latlon (default: CylindricalEquidistant)
- plot\_diff: draws difference plots (default: False)
- calc\_grading: calculates grading metrics (default: False)
- stippling: uses stippling to mark statistically significant differences (default: False = mask out non-significant differences in gray)
- show\_global\_avg: diplays the global avaerage of the input field as string at the top-right of lat-lon plots (default: False)
- annots: choose the annotation style, e.g. `alias` which would display the alias of the dataset as title (applies to plot\_type zonal and cycle\_zonal)
- metric: chosen grading metric(s) (if calc\_grading is True)
- normalization: metric normalization (for RMSD and BIAS metrics only)
- abs\_levs: list of contour levels for absolute plot
- diff\_levs: list of contour levels for difference plot
- zonal\_cmap: for plot\_type zonal only, chosen color table (default: "amwg\_blueyellowred")
- zonal\_ymin: for plot\_type zonal only, minimum pressure level on the y-axis (default: 5. hPa)
- latlon\_cmap: for plot\_type latlon only, chosen color table (default: "amwg\_blueyellowred")
- plot\_units: plotting units (if different from standard CMOR units)
- add\_tropopause: adds an outline of a climatological tropopause to the zonal plot (default: False)

#### Special optional plot configurations

It is possible to make some specific customizations to the plots (zonal only).

This includes for example specific tickmark labels of the axes.

Those special customizations can be done by adding ncl plotting resources combined with prefix res\_ as optional settings of the main script in the recipe.

Note that this requires to be familiar with the ncl plotting routines for pressure vs height plots (https://www.ncl. ucar.edu/Document/Graphics/Interfaces/gsn\_csm\_pres\_hgt.shtml) and the corresponding resources.

The following shows an example on customizing the latitude tickmarks so that a degree sign and and empty space is used for the labels:

Required settings (variables)

• reference\_dataset: reference dataset to compare with (usually the observations).

Optional settings (variables)

• alternative\_dataset: a second dataset to compare with.

These settings are passed to the other scripts by main.ncl, depending on the selected plot\_type.

1. Script collect.ncl

Required settings (scripts)

- metric: selected metric (RMSD, BIAS or taylor)
- · label\_bounds: for RMSD and BIAS metrics, min and max of the labelbar
- label\_scale: for RMSD and BIAS metrics, bin width of the labelbar
- · colormap: for RMSD and BIAS metrics, color table of the labelbar

Optional settings (scripts)

- label\_lo: adds lower triange for values outside range
- · label\_hi: adds upper triange for values outside range
- cm\_interval: min and max color of the color table
- cm\_reverse: reverses the color table
- sort: sorts datasets in alphabetic order (excluding MMM)
- diag\_order: sort diagnostics in a specific order (name = 'diagnostic'-'region')
- title: plots title
- scale\_font: scaling factor applied to the default font size
- disp\_values: switches on/off the grading values on the plot
- disp\_rankings: switches on/off the rankings on the plot
- rank\_order: displays rankings in increasing (1) or decreasing (-1) order

# 16.1.4 Variables

- 1. recipe\_perfmetrics\_CMIP5.yml
  - clt (atmos, monthly mean, longitude latitude time)
  - hus (atmos, monthly mean, longitude latitude lev time)
  - od550aer, od870aer, od550abs, od550lt1aer (aero, monthly mean, longitude latitude time)
  - pr (atmos, monthly mean, longitude latitude time)
  - rlut, rlutcs, rsut, rsutcs (atmos, monthly mean, longitude latitude time)
  - sm (land, monthly mean, longitude latitude time)
  - ta (atmos, monthly mean, longitude latitude lev time)
  - tas (atmos, monthly mean, longitude latitude time)
  - toz (atmos, monthly mean, longitude latitude time)
  - ts (atmos, monthly mean, longitude latitude time)
  - ua (atmos, monthly mean, longitude latitude lev time)
  - va (atmos, monthly mean, longitude latitude lev time)
  - zg (atmos, monthly mean, longitude latitude lev time)
- 2. recipe\_perfmetrics\_land\_CMIP5.yml
  - sm (land, monthly mean, longitude latitude time)
  - nbp (land, monthly mean, longitude latitude time)
  - gpp (land, monthly mean, longitude latitude time)
  - lai (land, monthly mean, longitude latitude time)
  - fgco2 (ocean, monthly mean, longitude latitude time)
  - et (land, monthly mean, longitude latitude time)
  - rlus, rlds, rsus, rdsd (atmos, monthly mean, longitude latitude time)

# 16.1.5 Observations and reformat scripts

The following list shows the currently used observational data sets for this recipe with their variable names and the reference to their respective reformat scripts in parentheses. Please note that obs4MIPs data can be used directly without any reformating. For non-obs4MIPs data use *esmvaltool data info DATASET* or see headers of cmorization scripts (in /esmvaltool/cmorizers/data/formatters/datasets/) for downloading and processing instructions. #. recipe\_perfmetrics\_CMIP5.yml

- AIRS (hus obs4MIPs)
- CERES-EBAF (rlut, rlutcs, rsut, rsutcs obs4MIPs)
- ERA-Interim (tas, ta, ua, va, zg, hus esmvaltool/cmorizers/data/formatters/datasets/era-interim.py)
- ESACCI-AEROSOL (od550aer, od870aer, od550abs, od550lt1aer esmvaltool/cmorizers/data/formatters/datasets/esacciaerosol.ncl)
- ESACCI-CLOUD (clt esmvaltool/cmorizers/data/formatters/datasets/esacci-cloud.ncl)
- ESACCI-OZONE (toz esmvaltool/cmorizers/data/formatters/datasets/esacci-ozone.ncl)

- ESACCI-SOILMOISTURE (sm esmvaltool/cmorizers/data/formatters/datasets/esacci\_soilmoisture.ncl)
- ESACCI-SST (ts esmvaltool/ucmorizers/data/formatters/datasets/esacci-sst.py)
- GPCP-SG (pr obs4MIPs)
- HadISST (ts esmvaltool/cmorizers/data/formatters/datasets/hadisst.ncl)
- MODIS (od550aer esmvaltool/cmorizers/data/formatters/datasets/modis.ncl)
- NCEP-NCAR-R1 (tas, ta, ua, va, zg esmvaltool/cmorizers/data/formatters/datasets/ncep\_ncar\_r1.py)
- NIWA-BS (toz esmvaltool/cmorizers/data/formatters/datasets/niwa\_bs.ncl)
- PATMOS-x (clt esmvaltool/cmorizers/data/formatters/datasets/patmos\_x.ncl)
- 1. recipe\_perfmetrics\_land\_CMIP5.yml
  - CERES-EBAF (rlus, rlds, rsus, rsds obs4MIPs)
  - ESACCI-SOILMOISTURE (sm esmvaltool/cmorizers/data/formatters/datasets/esacci\_soilmoisture.ncl)
  - FLUXCOM (gpp esmvaltool/cmorizers/data/formatters/datasets/fluxcom.py)
  - JMA-TRANSCOM (nbp, fgco2 esmvaltool/cmorizers/data/formatters/datasets/jma\_transcom.py)
  - LAI3d (lai esmvaltool/cmorizers/data/formatters/datasets/lai3g.py)
  - LandFlux-EVAL (et esmvaltool/cmorizers/data/formatters/datasets/landflux\_eval.py)
  - Landschuetzer2016 (fgco2 esmvaltool/cmorizers/data/formatters/datasets/landschuetzer2016.py)
  - MTE (gpp esmvaltool/cmorizers/data/formatters/datasets/mte.py)

# 16.1.6 References

- Gleckler, P. J., K. E. Taylor, and C. Doutriaux, Performance metrics for climate models, J. Geophys. Res., 113, D06104, doi: 10.1029/2007JD008972 (2008).
- Righi, M., Eyring, V., Klinger, C., Frank, F., Gottschaldt, K.-D., Jöckel, P., and Cionni, I.: Quantitative evaluation of oone and selected climate parameters in a set of EMAC simulations, Geosci. Model Dev., 8, 733, doi: 10.5194/gmd-8-733-2015 (2015).

# 16.1.7 Example plots

# **16.2 Single Model Performance Index (SMPI)**

## 16.2.1 Overview

This diagnostic calculates the Single Model Performance Index (SMPI) following Reichler and Kim (2008). The SMPI (called "I<sup>2</sup>") is based on the comparison of several different climate variables (atmospheric, surface and oceanic) between climate model simulations and observations or reanalyses, and it focuses on the validation of the time-mean state of climate. For I<sup>2</sup> to be determined, the differences between the climatological mean of each model variable and observations at each of the available data grid points are calculated, and scaled to the interannual variance from the validating observations. This interannual variability is determined by performing a bootstrapping method (random selection with replacement) for the creation of a large synthetic ensemble of observational climatologies. The results are then scaled to the average error from a reference ensemble of models, and in a final step the mean over all climate variables and one model is calculated. The plot shows the I<sup>2</sup> values for each model (orange circles) and the multimodel mean (black circle), with the diameter of each circle representing the range of I<sup>2</sup> values encompassed by the

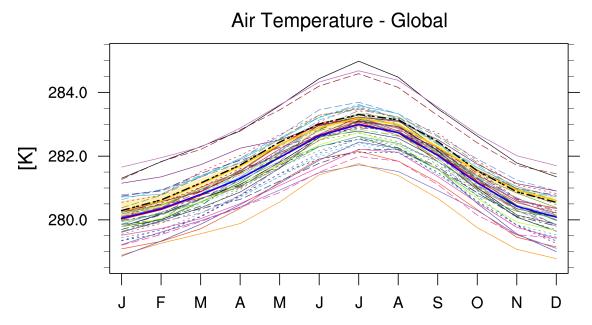


Fig. 1: Annual cycle of globally averaged temperature at 850 hPa (time period 1980-2005) for different CMIP5 models (historical simulation) (thin colored lines) in comparison to ERA-Interim (thick yellow line) and NCEP-NCAR-R1 (thick black dashed line) reanalysis data.

5th and 95th percentiles of the bootstrap ensemble. The  $I^2$  values vary around one, with values greater than one for underperforming models, and values less than one for more accurate models.

Note: The SMPI diagnostic needs all indicated variables from all added models for exactly the same time period to be calculated correctly. If one model does not provide a specific variable, either that model cannot be added to the SMPI calculations, or the missing variable has to be removed from the diagnostics all together.

# 16.2.2 Available recipes and diagnostics

Recipes are stored in recipes/

- recipe\_smpi.yml
- recipe\_smpi\_4cds.yml

Diagnostics are stored in diag\_scripts/perfmetrics/

- main.ncl: calculates and (optionally) plots annual/seasonal cycles, zonal means, lat-lon fields and time-lat-lon fields. The calculated fields can also be plotted as difference w.r.t. a given reference dataset. main.ncl also calculates RMSD, bias and taylor metrics. Input data have to be regridded to a common grid in the preprocessor. Each plot type is created by a separated routine, as detailed below.
- cycle\_zonal.ncl: calculates single model performance index (Reichler and Kim, 2008). It requires fields precalculated by main.ncl.
- collect.ncl: collects the metrics previously calculated by cycle\_latlon.ncl and passes them to the plotting functions.

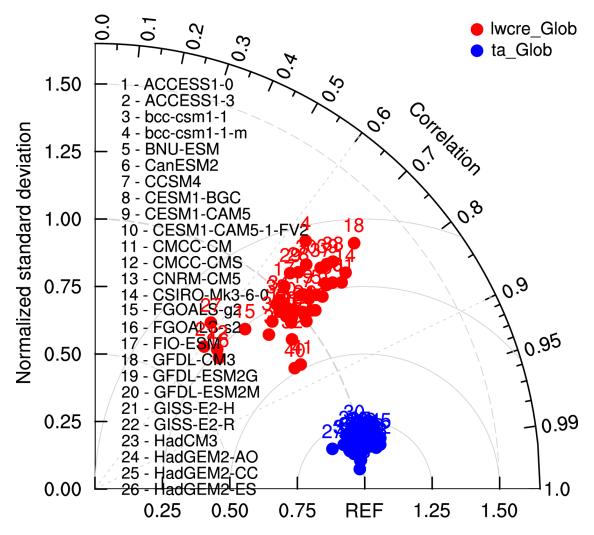


Fig. 2: Taylor diagram of globally averaged temperature at 850 hPa (ta) and longwave cloud radiative effect (lwcre) for different CMIP5 models (historical simulation, 1980-2005). Reference data (REF) are ERA-Interim for temperature (1980-2005) and CERES-EBAF (2001-2012) for longwave cloud radiative effect.

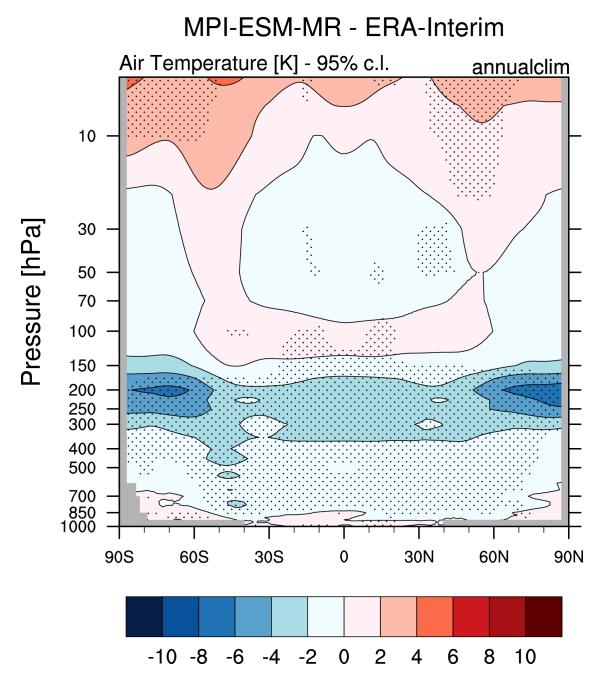
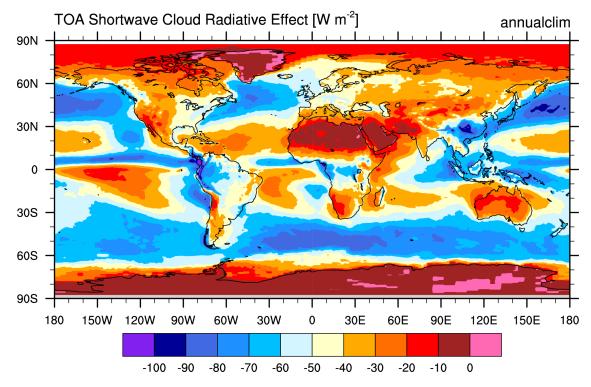


Fig. 3: Difference in annual mean of zonally averaged temperature (time period 1980-2005) between the CMIP5 model MPI-ESM-MR (historical simulation) and ERA-Interim. Stippled areas indicdate differences that are statistically significant at a 95% confidence level.



# **CERES-EBAF**

Fig. 4: Annual mean (2001-2012) of the shortwave cloud radiative effect from CERES-EBAF.

# 16.2.3 User settings

1. perfmetrics/main.ncl

Required settings for script

- plot\_type: only "cycle\_latlon (time, lat, lon)" and "cycle\_zonal (time, plev, lat)" available for SMPI; usage is defined in the recipe and is dependent on the used variable (2D variable: cycle\_latlon, 3D variable: cycle\_zonal)
- time\_avg: type of time average (only "yearly" allowed for SMPI, any other settings are not supported for this diagnostic)
- region: selected region (only "global" allowed for SMPI, any other settings are not supported for this diagnostic)
- normalization: metric normalization ("CMIP5" for analysis of CMIP5 simulations; to be adjusted accordingly for a different CMIP phase)
- calc\_grading: calculates grading metrics (has to be set to "true" in the recipe)
- metric: chosen grading metric(s) (if calc\_grading is True; has to be set to "SMPI")
- smpi\_n\_bootstrap: number of bootstrapping members used to determine uncertainties on model-reference differences (typical number of bootstrapping members: 100)

#### Required settings for variables

• reference\_dataset: reference dataset to compare with (usually the observations).

These settings are passed to the other scripts by main.ncl, depending on the selected plot\_type.

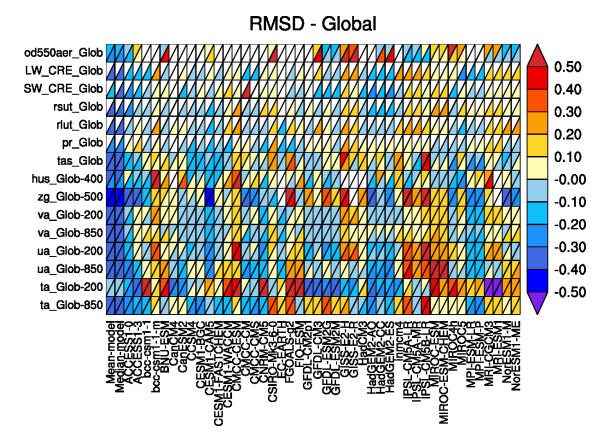


Fig. 5: Relative space-time root-mean-square deviation (RMSD) calculated from the climatological seasonal cycle of CMIP5 simulations. A relative performance is displayed, with blue shading indicating better and red shading indicating worse performance than the median of all model results. A diagonal split of a grid square shows the relative error with respect to the reference data set (lower right triangle) and the alternative data set (upper left triangle). White boxes are used when data are not available for a given model and variable.

- 1. collect.ncl
  - Required settings for script
    - metric: selected metric (has to be "SMPI")

## 16.2.4 Variables

- hfds (ocean, monthly mean, longitude latitude time)
- hus (atmos, monthly mean, longitude latitude lev time)
- pr (atmos, monthly mean, longitude latitude time)
- psl (atmos, monthly mean, longitude latitude time)
- sic (ocean-ice, monthly mean, longitude latitude time)
- ta (atmos, monthly mean, longitude latitude lev time)
- tas (atmos, monthly mean, longitude latitude time)
- tauu (atmos, monthly mean, longitude latitude time)
- tauv (atmos, monthly mean, longitude latitude time)
- tos (ocean, monthly mean, longitude latitude time)
- ua (atmos, monthly mean, longitude latitude lev time)
- va (atmos, monthly mean, longitude latitude lev time)

# 16.2.5 Observations and reformat scripts

The following list shows the currently used observational data sets for this recipe with their variable names and the reference to their respective reformat scripts in parentheses. Please note that obs4MIPs data can be used directly without any reformatting. For non-obs4MIPs data use *esmvaltool data info DATASET* or see headers of cmorization scripts for downloading and processing instructions.

- ERA-Interim (hfds, hus, psl, ta, tas, tauu, tauv, ua, va esmvaltool/data/formatters/datasets/era-interim.py)
- HadISST (sic, tos esmvaltool/data/formatters/datasets/hadisst.ncl)
- GPCP-V2.2 (pr obs4MIPs)

## 16.2.6 References

• Reichler, T. and J. Kim, How well do coupled models simulate today's climate? Bull. Amer. Meteor. Soc., 89, 303-311, doi: 10.1175/BAMS-89-3-303, 2008.

# 16.2.7 Example plots

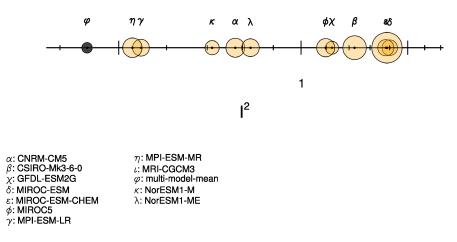


Fig. 6: Performance index  $I^2$  for individual models (circles). Circle sizes indicate the length of the 95% confidence intervals. The black circle indicates the  $I^2$  of the multi-model mean (similar to Reichler and Kim (2008), Figure 1).

# CHAPTER SEVENTEEN

# **FUTURE PROJECTIONS**

# 17.1 Climate model Weighting by Independence and Performance (ClimWIP)

## 17.1.1 Overview

Projections of future climate change are often based on multi-model ensembles of global climate models such as CMIP6. To condense the information from these models they are often combined into probabilistic estimates such as mean and a related uncertainty range (such as the standard deviation). However, not all models in a given multi-model ensemble are always equally 'fit for purpose' and it can make sense to weight models based on their ability to simulate observed quantities related to the target. In addition, multi-model ensembles, such as CMIP can contain several models based on a very similar code-base (sharing of components, only differences in resolution etc.) leading to complex inter-dependencies between the models. Adjusting for this by weighting models according to their independence helps to adjust for this.

This recipe implements the **Climate model Weighting by Independence and Performance (ClimWIP)** method. It is based on work by Knutti et al. (2017), Lorenz et al. (2018), Brunner et al. (2019), Merrifield et al. (2020), Brunner et al. (2020). Weights are calculated based on historical model performance in several metrics (which can be defined by the performance\_contributions parameter) as well as by their independence to all the other models in the ensemble based on their output fields in several metrics (which can be defined by the independence\_contributions parameter). These weights can be used in subsequent evaluation scripts (some of which are implemented as part of this diagnostic).

**Note**: this recipe is still being developed! A more comprehensive (yet older) implementation can be found on GitHub: https://github.com/lukasbrunner/ClimWIP

# 17.1.2 Using shapefiles for cutting scientific regions

To use shapefiles for selecting SREX or AR6 regions by name it is necessary to download them, e.g., from the sources below and reference the file using the *shapefile* parameter. This can either be a absolute or a relative path. In the example recipes they are stored in a subfolder *shapefiles* in the *auxiliary\_data\_dir* (with is specified in the config-user.yml).

SREX regions (AR5 reference regions): http://www.ipcc-data.org/guidelines/pages/ar5\_regions.html

AR6 reference regions: https://github.com/SantanderMetGroup/ATLAS/tree/v1.6/reference-regions

# 17.1.3 Available recipes and diagnostics

Recipes are stored in esmvaltool/recipes/

- recipe\_climwip\_test\_basic.yml: Basic sample recipe using only a few models
- recipe\_climwip\_test\_performance\_sigma.yml: Advanced sample recipe for testing the perfect model test in particular
- recipe\_climwip\_brunner2019\_med.yml: Slightly modified results for one region from Brunner et al. (2019) (to change regions see below)
- recipe\_climwip\_brunner2020esd.yml: Slightly modified results for Brunner et al. (2020)

Diagnostics are stored in esmvaltool/diag\_scripts/weighting/climwip/

- main.py: Compute weights for each input dataset
- calibrate\_sigmas.py: Compute the sigma values on the fly
- core\_functions.py: A collection of core functions used by the scripts
- io\_functions.py: A collection of input/output functions used by the scripts

Plot scripts are stored in esmvaltool/diag\_scripts/weighting/

- weighted\_temperature\_graph.py: Show the difference between weighted and non-weighted temperature anomalies as time series.
- weighted\_temperature\_map.py: Show the difference between weighted and non-weighted temperature anomalies on a map.
- plot\_utilities.py: A collection of functions used by the plot scripts.

# 17.1.4 User settings in recipe

1. Script main.py

**Required** settings for script

- performance\_sigma xor calibrate\_performance\_sigma: If performance\_contributions is given exactly one of the two has to be given. Otherwise they can be skipped or not set.
  - performance\_sigma: float setting the shape parameter for the performance weights calculation (determined offline).
  - calibrate\_performance\_sigma: dictionary setting the performance sigma calibration. Has to contain at least the key-value pair specifying target: variable\_group. Optional parameters for adjusting the calibration are not yet implemented. Warning: It is highly recommended to visually inspect the graphical output of the calibration to check if everything worked as intended. In case the calibration fails, the best performance sigma will still be indicated in the figure (see example Fig. 5 below) but not automatically picked - the user can decide to use it anyway by setting it in the recipe (not recommenced).
- independence\_sigma: float setting the shape parameter for the independence weights calculation (determined offline). Can be skipped or not set if independence\_contributions is skipped or not set. A on-the-fly calculation of the independence sigma is not yet implemented
- performance\_contributions: dictionary where the keys represent the variable groups to be included in the performance calculation. The values give the relative contribution of each group, with 0 being equivalent to not including the group. Can be skipped or not set

then weights will be based purely on model independence (this is mutually exclusive with independence\_contributions being skipped or not set).

- independence\_contributions: dictionary where the keys represent the variable groups to be included in the independence calculation. The values give the relative contribution of each group, with 0 being equivalent to not including the group. If skipped or not set weights will be based purely on model performance (this is mutually exclusive with performance\_contributions being skipped or not set).
- combine\_ensemble\_members: set to true if ensemble members of the same model should be combined during the processing (leads to identical weights for all ensemble members of the same model). Recommended if running with many (>10) ensemble members per model. If set to false, the model independence weighting will still (partly) account for the (very high) dependence between members of the same model. The success of this will depend on the case and the selected parameters. See Merrifield et al. (2020) for an in-depth discussion.
- obs\_data: list of project names to specify which are the observational data. The rest is assumed to be model data.

*Required settings for variables* \* This script takes multiple variables as input as long as they're available for all models \* start\_year: provide the period for which to compute performance and independence. \* end\_year: provide the period for which to compute performance and independence. \* mip: typically Amon \* preprocessor: e.g., climatological\_mean \* additional\_datasets: this should be \*obs\_data and is only needed for variables used in performance\_contributions.

#### **Required settings for preprocessor**

• Different combinations of preprocessor functions can be used, but the end result should always be aggregated over the time dimension, i.e. the input for the diagnostic script should be 2d (lat/lon).

#### **Optional settings for preprocessor**

- extract\_region or extract\_shape can be used to crop the input data.
- extract\_season can be used to focus on a single season.
- different climate statistics can be used to calculate mean, (detrended) std\_dev, or trend.
- 2. Script weighted\_temperature\_graph.py

#### **Required settings for script**

- ancestors: must include weights from previous diagnostic
- weights: the filename of the weights: 'weights.nc'
- settings: a list of plot settings: start\_year (integer), end\_year (integer), central\_estimate ('mean' or integer between 0 and 100 giving the percentile), lower\_bound (integer between 0 and 100), upper\_bound (integer between 0 and 100)

#### Required settings for variables

- This script only takes temperature (tas) as input
- start\_year: provide the period for which to plot a temperature change graph.
- end\_year: provide the period for which to plot a temperature change graph.
- mip: typically Amon
- preprocessor: temperature\_anomalies

#### Required settings for preprocessor

• Different combinations of preprocessor functions can be used, but the end result should always be aggregated over the latitude and longitude dimensions, i.e. the input for the diagnostic script should be 1d (time).

#### **Optional settings for preprocessor**

- Can be a global mean or focus on a point, region or shape
- · Anomalies can be calculated with respect to a custom reference period
- Monthly, annual or seasonal average/extraction can be used
- 3. Script weighted\_temperature\_map.py

#### **Required settings for script**

- ancestors: must include weights from previous diagnostic
- weights: the filename of the weights: 'weights\_combined.nc'

#### **Optional settings for script**

- model\_aggregation: how to aggregate the models: mean (default), median, integer between 0 and 100 representing a percentile
- xticks: positions to draw xticks at
- yticks: positions to draw yticks at

#### Required settings for variables

- This script takes temperature (tas) as input
- **start\_year**: provide the period for which to plot a temperature change graph.
- end\_year: provide the period for which to plot a temperature change graph.
- mip: typically Amon
- preprocessor: temperature\_anomalies

#### **Optional settings for variables**

- A second variable is optional: temperature reference (tas\_reference). If given, maps of temperature change to the reference are drawn, otherwise absolute temperatures are drawn.
- tas\_reference takes the same fields as tas

# 17.1.5 Updating the Brunner et al. (2019) recipe for new regions

recipe\_climwip\_brunner2019\_med.yml demonstrates a very similar setup to Brunner et al. (2019) but only for one region (the Mediterranean). To calculated weights for other regions the recipe needs to be updated in two places:

```
extract_shape:
    shapefile: shapefiles/srex.shp
    decomposed: True
    method: contains
    crop: true
    ids:
        - 'South Europe/Mediterranean [MED:13]'
```

The ids field takes any valid SREX region key or any valid AR6 region key (depending on the shapefile). Note that this needs to be the full string here (not the abbreviation).

The sigma parameters need to be set according to the selected region. The sigma values for the regions used in Brunner et al. (2019) can be found in table 1 of the paper.

```
performance_sigma: 0.546
independence_sigma: 0.643
```

**Warning:** if a new region is used the sigma values should be recalculated! This can be done by commenting out the sigma values (lines above) and commenting in the blocks defining the target of the weighting:

```
CLIM_future:
short_name: tas
start_year: 2081
end_year: 2100
mip: Amon
preprocessor: region_mean
```

as well as

```
calibrate_performance_sigma:
    target: CLIM_future
```

In this case ClimWIP will attempt to perform an on-the-fly perfect model test to estimate the lowest performance sigma (strongest weighting) which does not lead to overconfident weighting. **Important:** the user should always check the test output for unusual behaviour. For most cases the performance sigma should lie around 0.5. In cases where the perfect model test fails (no appropriate performance sigma can be found) the test will still produce graphical output before raising a ValueError. The user can then decide to manually set the performance sigma to the most appropriate value (based on the output) - **this is not recommended** and should only be done with care! The perfect model test failing can be a hint for one of the following: (1) not enough models in the ensemble for a robust distribution (normally >20 models should be used) or (2) the performance metrics used are not relevant for the target.

An on-the-fly calibration for the independence sigma is not yet implemented. For most cases we recommend to use the same setup as in Brunner et al. (2020) or Merrifield et al. (2020) (global or hemispherical temperature and sea level pressure climatologies as metrics and independence sigma values between 0.2 and 0.5).

**Warning:** if a new region or target is used the provided metrics to establish the weights might no longer be appropriate. Using unrelated metrics with no correlation and/or physical relation to the target will reduce the skill of the weighting and ultimately render it useless! In such cases the perfect model test might fail. This means the performance metrics should be updated.

# 17.1.6 Brunner et al. (2020) recipe and example independence weighting

recipe\_climwip\_brunner2020esd.yml implements the weighting used in Brunner et al. (2020). Compared to the paper there are minor differences due to two models which had to be excluded due to errors in the ESMValTool pre-processor: CAMS-CSM1-0 and MPI-ESM1-2-HR (r2) as well as the use of only one observational dataset (ERA5).

The recipe uses an additional step between pre-processor and weight calculation to calculate anomalies relative to the global mean (e.g., tas\_ANOM = tas\_CLIM - global\_mean(tas\_CLIM)). This means we do not use the absolute temperatures of a model as performance criterion but rather the horizontal temperature distribution (see Brunner et al. 2020 for a discussion).

This recipe also implements a somewhat general independence weighting for CMIP6. In contrast to model performance (which should be case specific) model independence can largely be seen as only dependent on the multi-model ensemble in use but not the target variable or region. This means that the configuration used should be valid for similar subsets of CMIP6 as used in this recipe:

combine\_ensemble\_members: true independence\_sigma: 0.54 independence\_contributions: tas\_CLIM\_i: 1 psl\_CLIM\_i: 1

Note that this approach weights ensemble members of the same model with a 1/N independence scaling (combine\_ensemble\_members: true) as well as different models with an output-based independence weighting. Different approaches to handle ensemble members are discussed in Merrifield et al. (2020). Note that, unlike for performance, climatologies are used for independence (i.e., the global mean is **not** removed for independence). **Warning:** Using only the independence weighting without any performance weighting might not always lead to meaningful results! The independence weighting is based on model output, which means that if a model is very different from all other models as well as the observations it will get a very high independence weight (and also total weight in absence of any performance weighting). This might not reflect the actual independence. It is therefore recommended to use weights based on both independence and performance for most cases.

# 17.1.7 Variables

- pr (atmos, monthly mean, longitude latitude time)
- tas (atmos, monthly mean, longitude latitude time)
- psl (atmos, monthly mean, longitude latitude time)
- rsus, rsds, rlus, rlds, rsns, rlns (atmos, monthly mean, longitude latitude time)
- more variables can be added if available for all datasets.

# 17.1.8 Observations and reformat scripts

Observation data is defined in a separate section in the recipe and may include multiple datasets.

# 17.1.9 References

- Brunner et al. (2020), Earth Syst. Dynam., 11, 995-1012
- Merrifield et al. (2020), Earth Syst. Dynam., 11, 807-834
- Brunner et al. (2019), Environ. Res. Lett., 14, 124010
- Lorenz et al. (2018), J. Geophys. Res.: Atmos., 9, 4509-4526
- Knutti et al. (2017), Geophys. Res. Lett., 44, 1909-1918

ACCESS1-0\_r1i1p1\_historical-rcp45 ACCESS1-0 r1i1p1 historical-rcp85 ACCESS1-3\_r1i1p1\_historical-rcp45 ACCESS1-3 r1i1p1 historical-rcp85 CanESM2\_r4i1p1\_historical-rcp45 -CanESM2 r3i1p1 historical-rcp45 -CanESM2\_r5i1p1\_historical-rcp45 CanESM2\_r2i1p1\_historical-rcp45 -CanESM2\_r1i1p1\_historical-rcp45 -CCSM4\_r1i1p1\_historical-rcp45 -CCSM4 r3i1p1 historical-rcp45 CCSM4\_r2i1p1\_historical-rcp45 -CCSM4\_r4i1p1\_historical-rcp45 -CCSM4\_r3i1p1\_historical-rcp60 CCSM4 r4i1p1 historical-rcp60 -CCSM4\_r1i1p1\_historical-rcp60 -CCSM4 r2i1p1 historical-rcp60 -CCSM4\_r4i1p1\_historical-rcp85 -CCSM4 r3i1p1 historical-rcp85 CCSM4\_r2i1p1\_historical-rcp85 -

CCSM4\_r1ilp1\_historical-rcp85 CSIRO-Mk3-6-0\_r9ilp1\_historical-rcp26 CSIRO-Mk3-6-0\_r3ilp1\_historical-rcp26 CSIRO-Mk3-6-0\_r3ilp1\_historical-rcp26 CSIRO-Mk3-6-0\_r5ilp1\_historical-rcp26 CSIRO-Mk3-6-0\_r8ilp1\_historical-rcp26 CSIRO-Mk3-6-0\_r2ilp1\_historical-rcp26 CSIRO-Mk3-6-0\_r101p1\_historical-rcp26 CSIRO-Mk3-6-0\_r101p1\_historical-rcp26 CSIRO-Mk3-6-0\_r11p1\_historical-rcp26 CSIRO-Mk3-6-0\_r11p1\_historical-rcp26 CSIRO-Mk3-6-0\_r11p1\_historical-rcp26 BNU-ESM\_r11p1\_historical-rcp26 BNU-ESM\_r111p1\_historical-rcp26

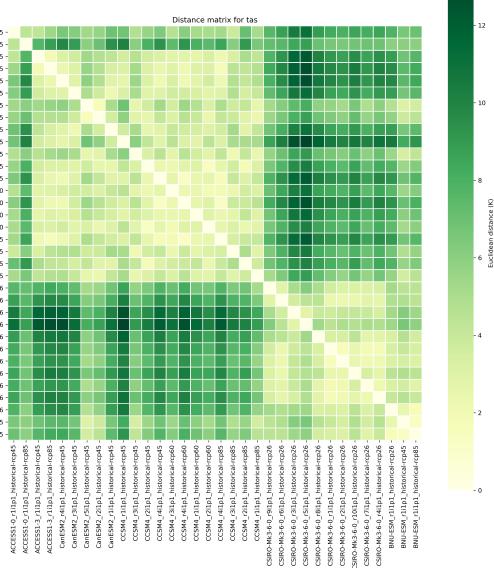


Fig. 1: Distance matrix for temperature, providing the independence metric.

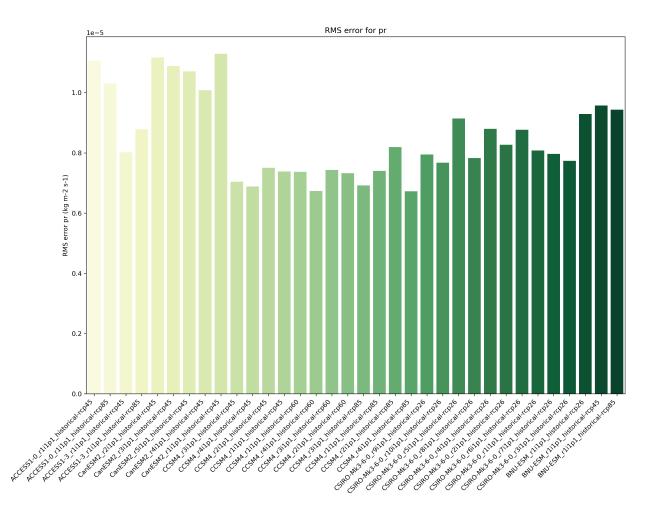


Fig. 2: Distance of preciptation relative to observations, providing the performance metric.

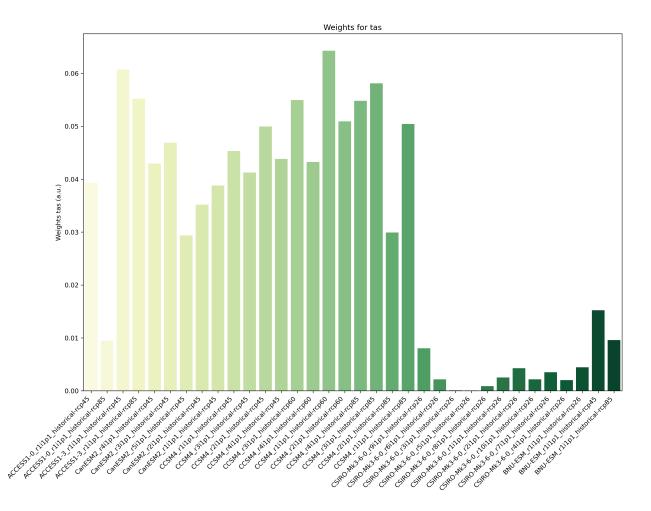


Fig. 3: Weights determined by combining independence and performance metrics for tas.

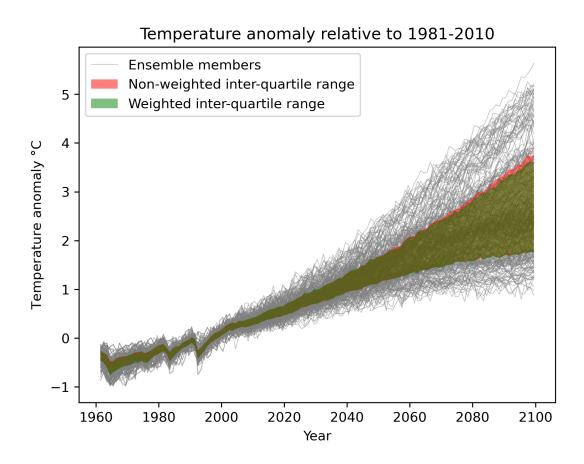


Fig. 4: Interquartile range of temperature anomalies relative to 1981-2010, weighted versus non-weighted.

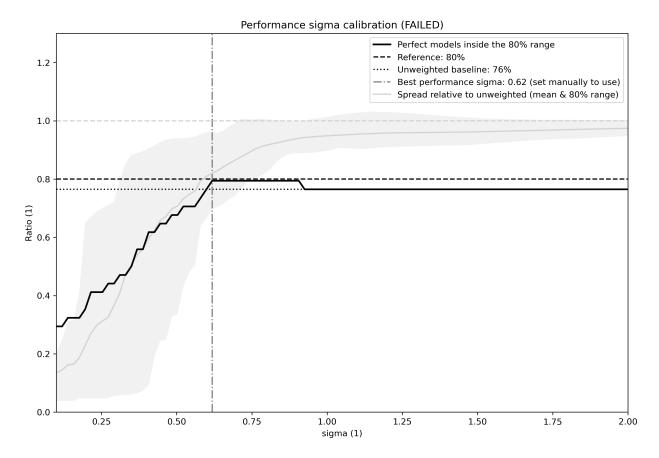


Fig. 5: Performance sigma calibration: The thick black line gives the reliability (c.f., weather forecast verification) which should reach at least 80%. The thick grey line gives the mean change in spread between the unweighted and weighted 80% ranges as an indication of the weighting strength (if it reaches 1, the weighting has no effect on uncertainty). The smallest sigma (i.e., strongest weighting) which is not overconfident (reliability  $\geq$  80%) is selected. If the test fails (like in this example) the smallest sigma which comes closest to 80% will be indicated in the legend (but NOT automatically selected).

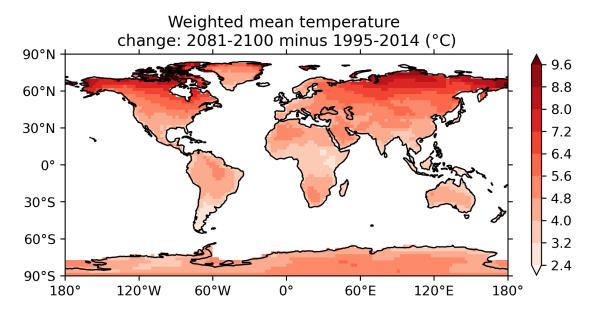


Fig. 6: Map of weighted mean temperature change 2081-2100 relative to 1995-2014

# 17.1.10 Example plots

# 17.2 Constraining future Indian Summer Monsoon projections with the present-day precipitation over the tropical western Pacific

# 17.2.1 Overview

Following Li et al. (2017) the change between present-day and future Indian Summer Monsoon (ISM) precipitation is constrained using the precipitation over the tropical western Pacific compared to a fixed, observed amount of 6 mm d<sup>-1</sup> from Global Precipitation Climatology Project (GPCP) (Adler et al., 2003) for 1980-2009. For CMIP6, historical data for 1980-2009 should be used. For CMIP5 historical data from 1980-2005 should be used, due to the length of the data sets. At the moment it is not possible to use a combined ['historical', 'rcp'] data set, because the diagnostic requires that a historical data set is given.

# 17.2.2 Available recipes and diagnostics

Recipes are stored in recipes/

recipe\_li17natcc.yml

Diagnostics are stored in diag\_scripts/

• emergent\_constraints/lif1f2.py

# 17.2.3 User settings in recipe

The recipe can be run with different CMIP5 and CMIP6 models. For each model, two experiments must be given: one historical run, possibly between 1980-2009 and one other model experiment. The user can choose the other model experiment, but it needs to be the same for all given models. The start and end year for the second data set can be choosen by the user, but should be consistent for all models (the same for future scenarios, the same length for other experiments). Different ensemble members are not possible, yet.

# 17.2.4 Variables

- *pr* (atmos, monthly, longitude, latitude, time)
- *ua* (atmos, monthly, longitude, latitude, plev, time)
- va (atmos, monthly, longitude, latitude, plev, time)
- *ts* (atmos, monthly, longitude, latitude, time)

# 17.2.5 Observations and reformat scripts

None

# 17.2.6 References

• Li, G., Xie, S. P., He, C., and Chen, Z. S.: Western Pacific emergent constraint lowers projected increase in Indian summer monsoon rainfall, Nat Clim Change, 7, 708-+, 2017

# 17.2.7 Example plots

# 17.3 Constraining uncertainty in projected gross primary production (GPP) with machine learning

Warning: Not all datasets necessary to run these recipes are available on ESGF. The following datasets are missing:

- Dataset: co2, Amon, CMIP5, HadGEM2-ES, esmHistorical, r1i1p1
- Dataset: gpp, Lmon, CMIP5, MIROC-ESM, esmFixClim1, r1i1p1
- Supplementary: sftlf, fx, CMIP5, MIROC-ESM, esmFixClim1, r0i0p0

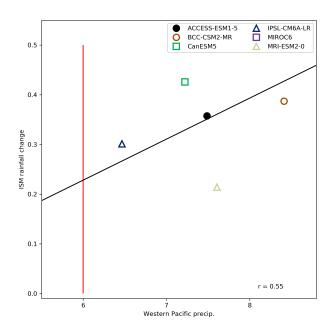


Fig. 7: Scatter plot of the simulated tropical western Pacific precipitation  $(mm d^{-1})$  versus projected average ISM (Indian Summer Monsoon) rainfall changes under the ssp585 scenario. The red line denotes the observed present-day western Pacific precipitation and the inter-model correlation (r) is shown. (CMIP6).

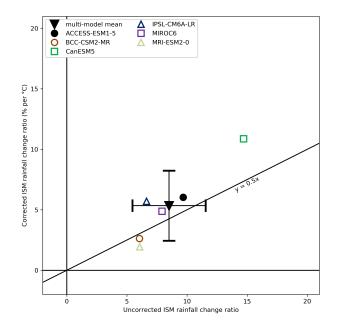


Fig. 8: Scatter plot of the uncorrected versus corrected average ISM (Indian Summer Monsoon) rainfall change ratios (% per degree Celsius of global SST warming). The error bars for the Multi-model mean indicate the standard deviation spread among models and the 2:1 line (y = 0.5x) is used to illustrate the Multi-model mean reduction in projected rainfall increase. (CMIP6).

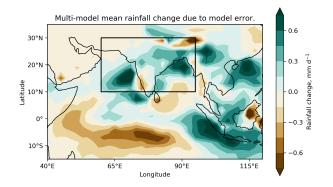


Fig. 9: Multi-model mean rainfall change due to model error. Box displays the area used to define the average ISM (Indian Summer Monsoon) rainfall. Precipitation changes are normalized by the corresponding global mean SST increase for each model. (CMIP6).

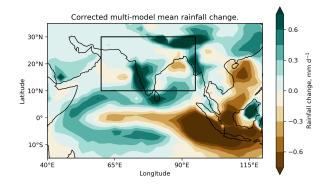


Fig. 10: Corrected multi-model mean rainfall change. Box displays the area used to define the average ISM (Indian Summer Monsoon) rainfall. Precipitation changes are normalized by the corresponding global mean SST increase for each model. (CMIP6).

# 17.3.1 Overview

These recipes reproduce the analysis of Schlund et al., JGR: Biogeosciences (2020). In this paper, a machine learning regression (MLR) approach (using the MLR algorithm Gradient Boosted Regression Trees, GBRT) is proposed to constrain uncertainties in projected gross primary production (GPP) in the RCP 8.5 scenario using observations of process-based diagnostics.

# 17.3.2 Available recipes and diagnostics

Recipes are stored in recipes/

- schlund20jgr/recipe\_schlund20jgr\_gpp\_abs\_rcp85.yml
- schlund20jgr/recipe\_schlund20jgr\_gpp\_change\_1pct.yml
- schlund20jgr/recipe\_schlund20jgr\_gpp\_change\_rcp85.yml

Diagnostics are stored in diag\_scripts/

• mlr/evaluate residuals.py

- mlr/main.py
- mlr/mmm.py
- *mlr/plot.py*
- mlr/postprocess.py
- mlr/preprocess.py
- mlr/rescale\_with\_emergent\_constraint.py

General information (including an example and more details) on machine learning regression (MLR) diagnostics is given *here*. The API documentation is available *here*.

# 17.3.3 Variables

- *co2s* (atmos, monthly, longitude, latitude, time)
- *gpp* (land, monthly, longitude, latitude, time)
- *gppStderr* (land, monthly, longitude, latitude, time)
- *lai* (land, monthly, longitude, latitude, time)
- pr (atmos, monthly, longitude, latitude, time)
- *rsds* (atmos, monthly, longitude, latitude, time)
- tas (atmos, monthly, longitude, latitude, time)

# 17.3.4 Observations and reformat scripts

- CRU (*pr*, *tas*)
- ERA-Interim (*rsds*)
- LAI3g (lai)
- MTE (gpp, gppStderr)
- Scripps-CO2-KUM (co2s)

# 17.3.5 References

• Schlund, M., Eyring, V., Camps-Valls, G., Friedlingstein, P., Gentine, P., & Reichstein, M. (2020). Constraining uncertainty in projected gross primary production with machine learning. Journal of Geophysical Research: Biogeosciences, 125, e2019JG005619, https://doi.org/10.1029/2019JG005619.

# 17.3.6 Example plots

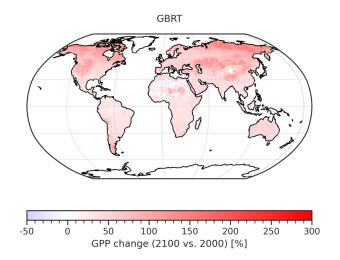


Fig. 11: GBRT-based prediction of the fractional GPP change over the 21st century (= GPP(2091-2100) / GPP(1991-2000)).

# 17.4 Context for interpreting equilibrium climate sensitivity and transient climate response from the CMIP6 Earth system models

# 17.4.1 Overview

This recipe reproduces the analysis of Meehl et al., Sci. Adv. (2020). In this paper, the equilibrium climate sensitivity (ECS) and transient climate response (TCR) are evaluated for the CMIP6 models and put into historical context.

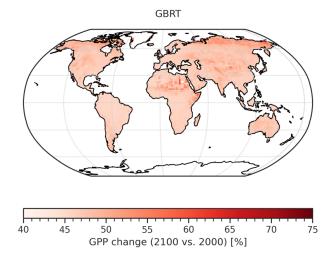


Fig. 12: Corresponding error of the GBRT-based prediction of the fractional GPP change over the 21st century (considering errors in the MLR model and errors in the predictors).

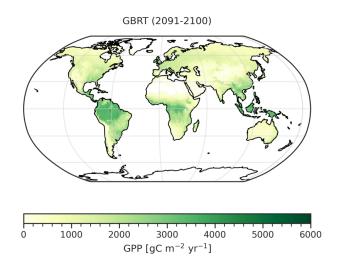


Fig. 13: GBRT-based prediction of the absolute GPP at the end of the 21st century (2091-2100).

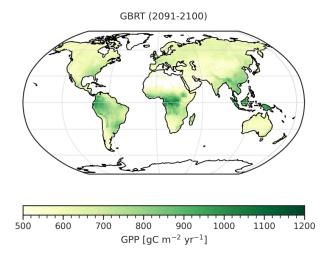


Fig. 14: Corresponding error of the GBRT-based prediction of the absolute GPP at the end of the 21st century (considering errors in the MLR model and errors in the predictors).

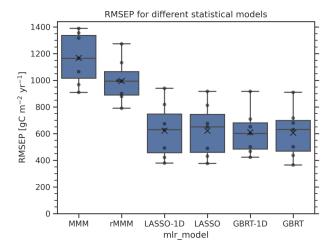


Fig. 15: Boxplot of the root mean square error of prediction (RMSEP) distributions for six different statistical models used to predict future absolute GPP (2091-2100) using a leave-one-model-out cross-validation approach. The distribution for each statistical model contains seven points (black dots, one for each climate model used as truth) and is represented in the following way: the lower and upper limit of the blue boxes correspond to the 25% and 75% quantiles, respectively. The central line in the box shows the median, the black "x" the mean of the distribution. The whiskers outside the box represent the range of the distribution

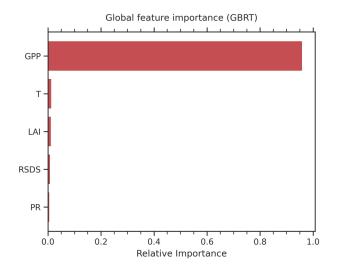


Fig. 16: Global feature importance of the GBRT model for prediction of the absolute GPP at the end of the 21st century (2091-2100).

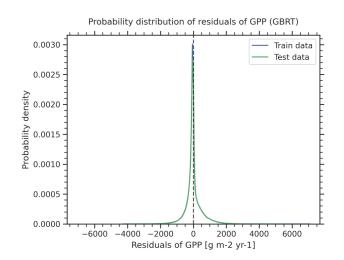


Fig. 17: Distribution of the residuals of the GBRT model for the prediction of absolute GPP at the end of the 21st century (2091-2100) for the training data (blue) and test data excluded from training (green).

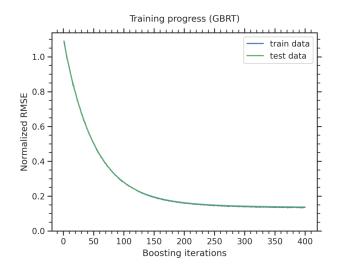


Fig. 18: Training progress of the GBRT model for the prediction of absolute GPP at the end of the 21st century (2091-2100) evaluated as normalized root mean square error on the training data (blue) and test data excluded from training (green).

# 17.4.2 Available recipes and diagnostics

Recipes are stored in recipes/

recipe\_meehl20sciadv.yml

Diagnostics are stored in diag\_scripts/

- climate\_metrics/ecs.py
- climate\_metrics/tcr.py
- climate\_metrics/create\_table.py
- ipcc\_ar5/ch09\_fig09\_42b.py

# 17.4.3 User settings in recipe

Script climate\_metrics/ecs.py

See *here*.

• Script climate\_metrics/tcr.py

See *here*.

- Script climate\_metrics/create\_table.py
  - calculate\_mean, *bool*, optional (default: True): Calculate mean over all datasets and add it to table.
  - calculate\_std, *bool*, optional (default: True): Calculate standard deviation over all datasets and add it to table.
  - exclude\_datasets, *list of str*, optional (default: ['MultiModelMean']): Exclude certain datasets when calculating statistics over all datasets and for assigning an index.
  - patterns, list of str, optional: Patterns to filter list of input data.
  - round\_output, *int*, optional: If given, round output to given number of decimals.

• Script ipcc\_ar5/ch09\_fig09\_42b.py See *here*.

### 17.4.4 Variables

- *rlut* (atmos, monthly, longitude, latitude, time)
- *rsdt* (atmos, monthly, longitude, latitude, time)
- rsut (atmos, monthly, longitude, latitude, time)
- tas (atmos, monthly, longitude, latitude, time)

## 17.4.5 References

• Meehl, G. A., Senior, C. A., Eyring, V., Flato, G., Lamarque, J. F., Stouffer, R. J., Taylor, K. E. and Schlund, M., *Context for interpreting equilibrium climate sensitivity and transient climate response from the CMIP6 Earth system models*, Science Advances, 6(26), eaba1981, https://doi.org/10.1126/sciadv.aba1981, 2020.

# 17.4.6 Example plots

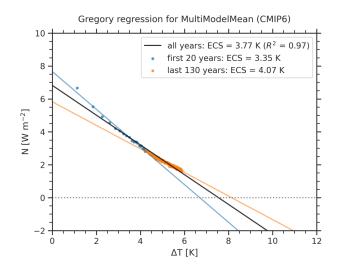


Fig. 19: ECS calculated for the CMIP6 models using the Gregory method over different time scales. Using the entire 150-year 4xCO2 experiment (black line), there is an ECS value of 3.8 K; using only the first 20 years (blue dots and blue line), there is an ECS of 3.4 K; and using the last 130 years, there is an ECS of 4.1 K (orange dots and orange line).

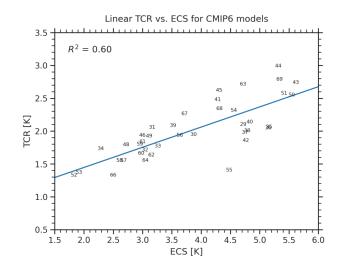


Fig. 20: TCR as a function of ECS for the CMIP6 models (black line is a linear fit). The  $R^2$  values are given in the upper left parts of each panel. The numbers denote individual CMIP6 models.

# 17.5 Emergent constraints for equilibrium climate sensitivity

## 17.5.1 Overview

Calculates equilibrium climate sensitivity (ECS) versus

- 1) S index, D index and lower tropospheric mixing index (LTMI); similar to fig. 5 from Sherwood et al. (2014)
- southern ITCZ index and tropical mid-tropospheric humidity asymmetry index; similar to fig. 2 and 4 from Tian (2015)
- 3) covariance of shortwave cloud reflection (Brient and Schneider, 2016)
- 4) climatological Hadley cell extent (Lipat et al., 2017)
- 5) temperature variability metric; similar to fig. 2 from Cox et al. (2018)
- 6) total cloud fraction difference between tropics and mid-latitudes; similar to fig. 3 from Volodin (2008)
- 7) response of marine boundary layer cloud (MBLC) fraction changes to sea surface temperature (SST); similar to fig. 3 of Zhai et al. (2015)
- 8) Cloud shallowness index (Brient et al., 2016)
- 9) Error in vertically-resolved tropospheric zonal average relative humidity (Su et al., 2014)

The results are displayed as scatterplots.

**Note:** The recipe recipe\_ecs\_scatter.yml requires pre-calulation of the equilibrium climate sensitivites (ECS) for all models. The ECS values are calculated with recipe\_ecs.yml. The netcdf file containing the ECS values (path and filename) is specified by diag\_script\_info@ecs\_file. Alternatively, the netcdf file containing the ECS values can be generated with the cdl-script \$diag\_scripts/emergent\_constraints/ecs\_cmip.cdl (recommended method):

- 1) save script given at the end of this recipe as ecs\_cmip.cdl
- 2) run command: ncgen -o ecs\_cmip.nc ecs\_cmip.cdl

3) copy ecs\_cmip.nc to directory given by diag\_script\_info@ecs\_file (e.g. \$diag\_scripts/emergent\_constraints/ecs\_cmip.nc)

# 17.5.2 Available recipes and diagnostics

Recipes are stored in recipes/

- recipe\_ecs\_scatter.yml
- recipe\_ecs\_constraints.yml

Diagnostics are stored in diag\_scripts

- emergent\_constraints/ecs\_scatter.ncl: calculate emergent constraints for ECS
- emergent\_constraints/ecs\_scatter.py: calculate further emergent constraints for ECS
- emergent\_constraints/single\_constraint.py: create scatterplots for emergent constraints
- climate\_metrics/psi.py: calculate temperature variabililty metric (Cox et al., 2018)

## 17.5.3 User settings in recipe

• Script emergent\_constraints/ecs\_scatter.ncl

Required settings (scripts)

- diag: emergent constraint to calculate ("itczidx", "humidx", "ltmi", "covrefl", "shhc", "sherwood\_d", "sherwood\_s")
- ecs\_file: path and filename of netCDF containing precalculated ECS values (see note above)

Optional settings (scripts)

- calcmm: calculate multi-model mean (True, False)
- legend\_outside: plot legend outside of scatterplots (True, False)
- output\_diag\_only: Only write netcdf files for X axis (True) or write all plots (False)
- output\_models\_only: Only write models (no reference datasets) to netcdf files (True, False)
- output\_attributes: Additonal attributes for all output netcdf files
- predef\_minmax: use predefined internal min/max values for axes (True, False)
- styleset: "CMIP5" (if not set, diagnostic will create a color table and symbols for plotting)
- suffix: string to add to output filenames (e.g."cmip3")

Required settings (variables)

- reference\_dataset: name of reference data set

```
Optional settings (variables)
```

none

Color tables

none

• Script emergent\_constraints/ecs\_scatter.py

See *here*.

- Script emergent\_constraints/single\_constraint.py
  - See here.
- Script climate\_metrics/psi.py

See here.

## 17.5.4 Variables

- cl (atmos, monthly mean, longitude latitude level time)
- clt (atmos, monthly mean, longitude latitude time)
- pr (atmos, monthly mean, longitude latitude time)
- hur (atmos, monthly mean, longitude latitude level time)
- hus (atmos, monthly mean, longitude latitude level time)
- rsdt (atmos, monthly mean, longitude latitude time)
- rsut (atmos, monthly mean, longitude latitude time)
- rsutcs (atmos, monthly mean, longitude latitude time)
- rtnt or rtmt (atmos, monthly mean, longitude latitude time)
- ta (atmos, monthly mean, longitude latitude level time)
- tas (atmos, monthly mean, longitude latitude time)
- tasa (atmos, monthly mean, longitude latitude time)
- tos (atmos, monthly mean, longitude latitude time)
- ts (atmos, monthly mean, longitude latitude time)
- va (atmos, monthly mean, longitude latitude level time)
- wap (atmos, monthly mean, longitude latitude level time)
- zg (atmos, monthly mean, longitude latitude time)

## 17.5.5 Observations and reformat scripts

#### Note:

- (1) Obs4mips data can be used directly without any preprocessing.
- (2) See headers of reformat scripts for non-obs4MIPs data for download instructions.
  - AIRS (obs4MIPs): hus, husStderr
  - AIRS-2-0 (obs4MIPs): hur
  - CERES-EBAF (obs4MIPs): rsdt, rsut, rsutcs
  - ERA-Interim (OBS6): hur, ta, va, wap
  - GPCP-SG (obs4MIPs): pr
  - HadCRUT4 (OBS): tasa

- HadISST (OBS): ts
- MLS-AURA (OBS6): hur
- TRMM-L3 (obs4MIPs): pr, prStderr

#### 17.5.6 References

- Brient, F., and T. Schneider, J. Climate, 29, 5821-5835, doi:10.1175/JCLIM-D-15-0897.1, 2016.
- Brient et al., Clim. Dyn., 47, doi:10.1007/s00382-015-2846-0, 2016.
- Cox et al., Nature, 553, doi:10.1038/nature25450, 2018.
- Gregory et al., Geophys. Res. Lett., 31, doi:10.1029/2003GL018747, 2004.
- Lipat et al., Geophys. Res. Lett., 44, 5739-5748, doi:10.1002/2017GL73151, 2017.
- Sherwood et al., nature, 505, 37-42, doi:10.1038/nature12829, 2014.
- Su, et al., J. Geophys. Res. Atmos., 119, doi:10.1002/2014JD021642, 2014.
- Tian, Geophys. Res. Lett., 42, 4133-4141, doi:10.1002/2015GL064119, 2015.
- Volodin, Izvestiya, Atmospheric and Oceanic Physics, 44, 288-299, doi:10.1134/S0001433808030043, 2008.
- Zhai, et al., Geophys. Res. Lett., 42, doi:10.1002/2015GL065911, 2015.

## 17.5.7 Example plots

## 17.6 Emergent constraints on carbon cycle feedbacks

#### 17.6.1 Overview

Figures from Wenzel et al. (2014) are reproduced with recipe\_wenzel14jgr.yml. Variables relevant for the carbon cycle - climate feedback such as near surface air temperature (tas), net biosphere productivity (nbp) and carbon flux into the ocean (fgco2) are analyzed for coupled (1pctCO2, here the carbon cycle is fully coupled to the climate response) and uncoupled (esmFixCLim1, here the carbon cycle is uncoupled to the climate response) simulations. The standard namelist includes a comparison of cumulated nbp from coupled and uncoupled simulations and includes a set of routines to diagnose the long-term carbon cycle - climate feedback parameter (GammaLT) from an ensemble of CMIP5 models. Also included in the recipe is a comparison of the interannual variability of nbp and fgco2 for historical simulations used to diagnose the observable sensitivity of CO2 to tropical temperature changes (GammaIAV). As a key figure of this recipe, the diagnosed values from the models GammaLT vs. GammaIAV are compared in a scatter plot constituting an emergent constraint.

## 17.6.2 Available recipes and diagnostics

Recipes are stored in recipes/

• recipe\_wenzel14jgr.yml

Diagnostics are stored in diag\_scripts/

- carbon\_tsline.ncl: time line plots of annual means for spatial averages
- carbon\_gammaHist.ncl: scatter plot of annual mean anomalies of two different variables; diagnosing and saving GammaIAV

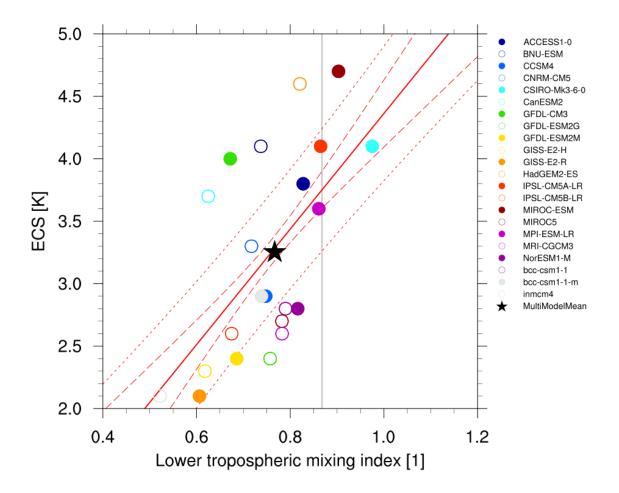


Fig. 21: Lower tropospheric mixing index (LTMI; Sherwood et al., 2014) vs. equilibrium climate sensitivity from CMIP5 models.

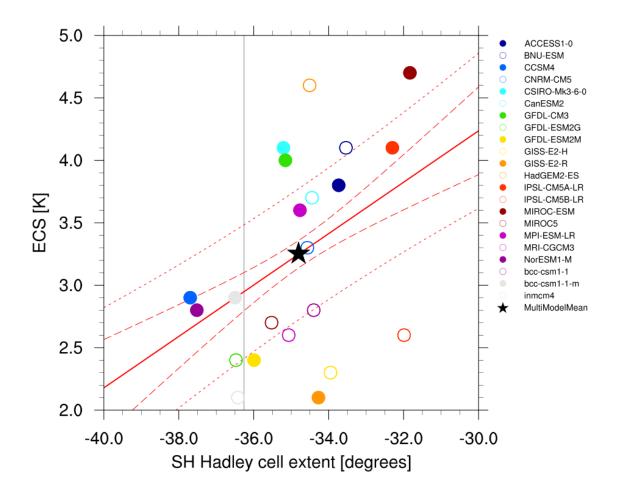


Fig. 22: Climatological Hadley cell extent (Lipat et al., 2017) vs. equilibrium climate sensitivity from CMIP5 models.

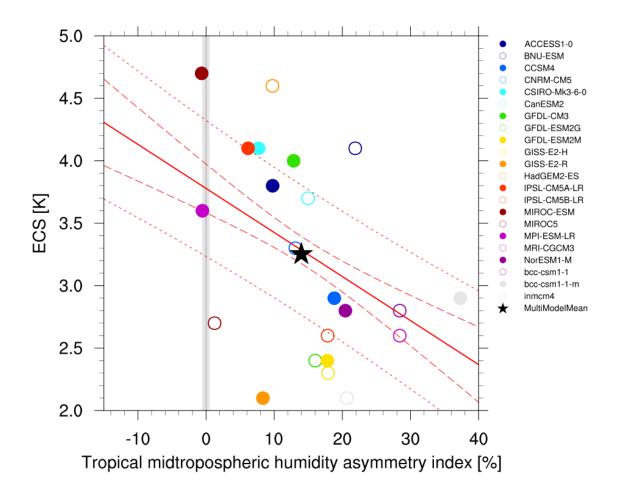


Fig. 23: Tropical mid-tropospheric humidity asymmetry index (Tian, 2015) vs. equilibrium climate sensitivity from CMIP5 models.

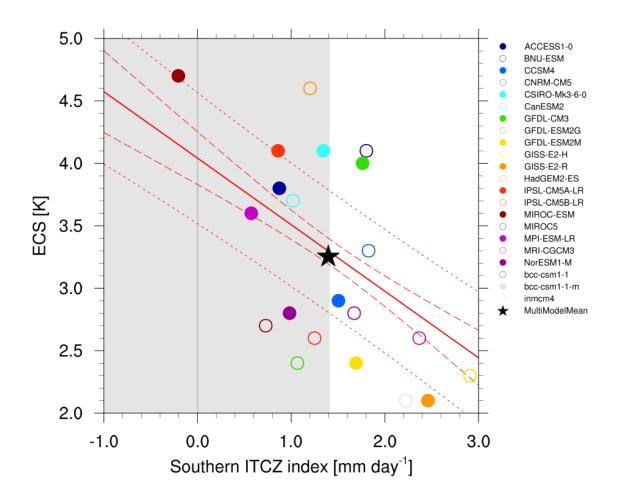


Fig. 24: Southern ITCZ index (Tian, 2015) vs. equilibrium climate sensitivity from CMIP5 models.

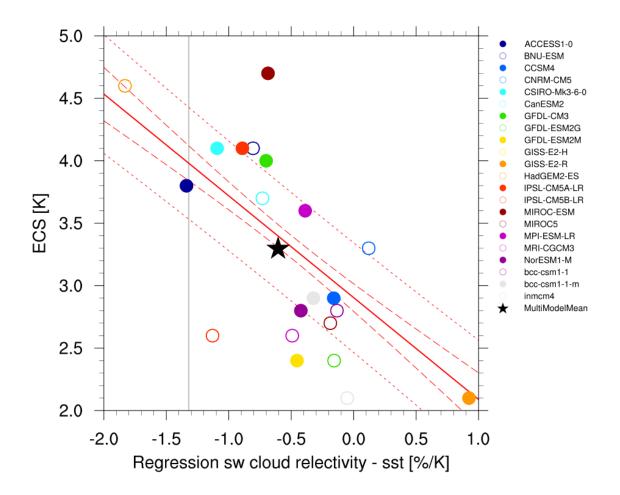


Fig. 25: Covariance of shortwave cloud reflection (Brient and Schneider, 2016) vs. equilibrium climate sensitivity from CMIP5 models.

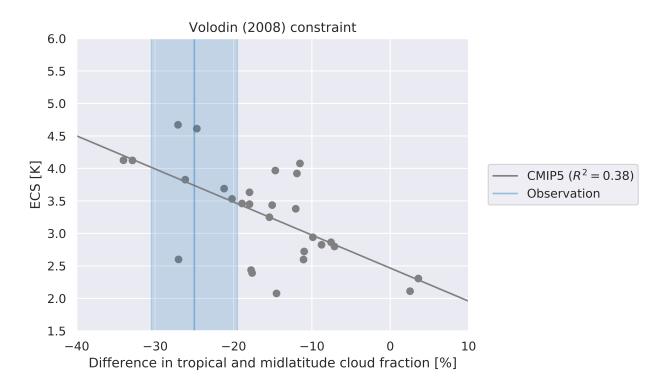


Fig. 26: Difference in total cloud fraction between tropics  $(28^{\circ}S - 28^{\circ}N)$  and Southern midlatitudes  $(56^{\circ}S - 36^{\circ}S)$  (Volodin, 2008) vs. equilibrium climate sensitivity from CMIP5 models.

• carbon\_constraint.ncl: scatter plot of GammaLT vs. GammaIAV + line plot of probability density functions, diagnosing GammaLT

## 17.6.3 User settings

**Note:** Make sure to run this recipe setting max\_parallel\_tasks: 1 in the config\_user.yml file or using the CLI flag --max\_parallel\_tasks=1.

User setting files (cfg files) are stored in nml/cfg\_carbon/

1. carbon\_tsline

Required Settings (scripts)

- ts\_minlat: minimum latitude for area averaging
- ts\_maxlat: maximum latitude for area averaging
- ts\_minlon: minimum longitude for area averaging
- ts\_maxlon: maximum longitude for area averaging
- ts\_maxyear: last year (time range)
- ts\_minyear: first year (time range)
- plot\_units: units to appear on Figure
- time\_avg: currently, only yearly is available

- area\_opper: type of area operation (sum)
- styleset: Plot style

Optional settings (scripts)

- multi\_model\_mean: True for multi-model mean calculation
- volcanoes: True for marking years with lage volcanic eruptions
- align: True for aligning models to have the same start year (needed for idealized 2x CO2 simulations)
- ts\_anomaly: calculates anomalies with respect to a defined time range average (anom)
- ridx\_start: if ts\_anomaly is True, define start time index for reference period
- ridx\_end: if ts\_anomaly is True, define end time index for reference period
- ref\_start: if ts\_anomaly is True, define start year for reference period
- ref\_end: if ts\_anomaly is True, define end year for reference period

#### Required settings (variables)

• reference\_dataset: name of reference data set

2. carbon\_gammaHist.ncl

Required Settings (scripts)

- start\_year: first year (time range)
- end\_year: last year (time range)
- plot\_units: units to appear on Figure
- ec\_anom: calculates anomalies with respect to the first 10-year average (anom)
- scatter\_log: set logarithmic axes in scatterplot.ncl
- styleset: Plot style

Optional settings (scripts)

- ec\_volc : exclude 2 years after volcanic erruptions (True/False)
- 3. carbon\_constraint.ncl

Required Settings (scripts)

- gIAV\_diagscript: "gammaHist\_Fig3and4"
- gIAV\_start: start year of GammIAV calculation period
- gIAV\_end: end year of GammIAV calculation period
- ec\_anom: True
- con\_units: label string for units, e.g. (GtC/K)
- nc\_infile: specify path to historical gamma values derived by carbon\_gammaHist.ncl
- styleset: Plot style

Optional settings (scripts)

• reg\_models: Explicit naming of individual models to be excluded from the regression

#### 17.6.4 Variables

- tas (atmos, monthly mean, longitude latitude time)
- nbp (land, monthly mean, longitude latitude time)
- fgco2 (ocean, monthly mean, longitude latitude time)

#### 17.6.5 Observations and reformat scripts

- GCP2018: Global Carbon Budget including land (nbp) and ocean (fgco2) carbon fluxes
- NCEP-NCAR-R1: National Centers for Environmental Prediction reanalysis data for near surface temperature

#### 17.6.6 References

- Cox, P. M., D. B. Pearson, B. B. Booth, P. Friedlingstein, C. C. Huntingford, C. D. B. Jones, and C. M. Luke, 2013, Sensitivity of tropical carbon to climate change constrained by carbon dioxide variability, Nature, 494(7437), 341-344. doi: 10.1038/nature11882
- Wenzel, S., P. M. Cox, V. Eyring, and P. Friedlingstein, 2014, Emergent Constraints on Climate Carbon Cycle Feedbacks in the CMIP5 Earth System Models, JGR Biogeoscience, 119(5), doi: 2013JG002591.

#### 17.6.7 Example plots

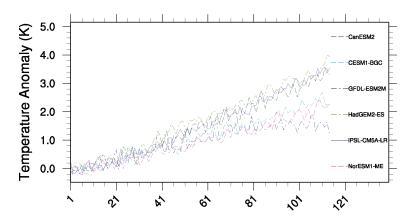


Fig. 27: Time series of tropical (30S to 30N) mean near surface temperature (tas) change between year 30 and year 110 for the CMIP5 models simulated with prescribed CO2 (1%/yr CO2 increase) coupled simulation (1pctCO2).

# 17.7 Emergent constraints on equilibrium climate sensitivity in CMIP5: do they hold for CMIP6?

#### 17.7.1 Overview

This recipe reproduces the analysis of Schlund et al., Earth Sys. Dyn. (2020). In this paper, emergent constraints on the equilibrium climate sensitivity are evaluated on CMIP5 and CMIP6 models. Since none of the considered emergent constraints have been developed on the CMIP6 ensemble, this allows an out-of-sample testing of the emergent constraints. Most emergent constraints show a reduced skill in CMIP6 when compared to CMIP5.

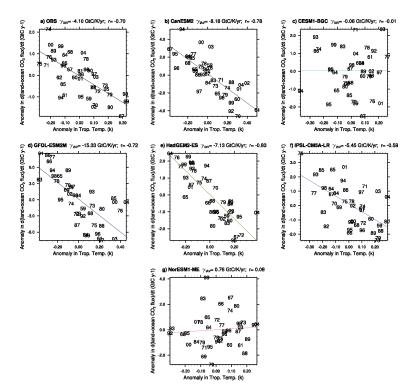


Fig. 28: Correlations between the interannual variability of global co2flux (nbp+fgco2) and tropical temperature for the individual CMIP5 models using esmHistorical simulations, and for observations.

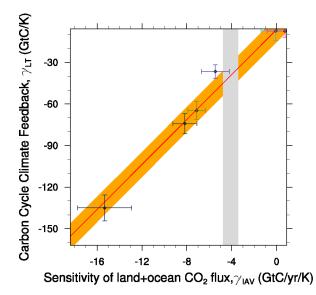


Fig. 29: Carbon cycle-climate feedback of tropical land carbon vs. the sensitivity of co2flux to interannual temperature variability in the tropics (30S to 30N). The red line shows the linear best fit of the regression together with the prediction error (orange shading) and the gray shading shows the observed range.

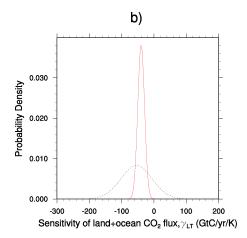


Fig. 30: Probability Density Functions for the pure CMIP5 ensemble (black dashed) and after applying the observed constraint to the models (red solid)

## 17.7.2 Available recipes and diagnostics

Recipes are stored in recipes/

• recipe\_schlund20esd.yml

Diagnostics are stored in diag\_scripts/

- climate\_metrics/ecs.py
- climate\_metrics/psi.py
- emergent\_constraints/ecs\_scatter.ncl
- emergent\_constraints/ecs\_scatter.py
- emergent\_constraints/multiple\_constraints.py

More details on the emergent constraint module are given in the API documentation which is available here.

## 17.7.3 Variables

- *cl* (atmos, monthly, longitude, latitude, level, time)
- *clt* (atmos, monthly, longitude, latitude, time)
- *hur* (atmos, monthly, longitude, latitude, level, time)
- hus (atmos, monthly, longitude, latitude, level, time)
- pr (atmos, monthly, longitude, latitude, time)
- *rsdt* (atmos, monthly, longitude, latitude, time)
- *rsut* (atmos, monthly, longitude, latitude, time)
- *rsutcs* (atmos, monthly, longitude, latitude, time)
- rtnt or rtmt (atmos, monthly, longitude, latitude, time)
- *ta* (atmos, monthly, longitude, latitude, level, time)
- tas (atmos, monthly, longitude, latitude, time)

- tasa (atmos, monthly, longitude, latitude, time)
- tos (atmos, monthly, longitude, latitude, time)
- *ts* (atmos, monthly, longitude, latitude, time)
- va (atmos, monthly, longitude, latitude, level, time)
- wap (atmos, monthly, longitude, latitude, level, time)

## 17.7.4 Observations and reformat scripts

- AIRS (hur, hus)
- CERES-EBAF (rsut, rsutcs, rsdt)
- ERA-Interim (hur, ta, va, wap)
- GPCP-SG (pr)
- HadCRUT4 (tasa)
- HadISST (ts)
- MLS-AURA (hur)

## 17.7.5 References

• Schlund, M., Lauer, A., Gentine, P., Sherwood, S. C., and Eyring, V.: Emergent constraints on equilibrium climate sensitivity in CMIP5: do they hold for CMIP6?, Earth Syst. Dynam., 11, 1233–1258, https://doi.org/10. 5194/esd-11-1233-2020, 2020.

## 17.7.6 Example plots

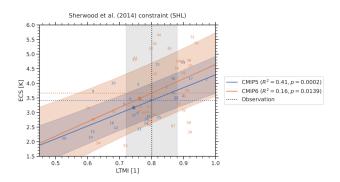


Fig. 31: Emergent relationship (solid blue and orange lines) of the Sherwood et al. (2014) emergent constraint, which is based on the lower tropospheric mixing index (LTMI). The numbers correspond to individual CMIP models. The shaded area around the regression line corresponds to the standard prediction error, which defines the error in the regression model itself. The vertical dashed black line corresponds to the observational reference with its uncertainty range given as standard error (gray shaded area). The horizontal dashed lines show the best estimates of the constrained ECS for CMIP5 (blue) and CMIP6 (orange). The colored dots mark the CMIP5 (blue) and CMIP6 (orange) multi-model means.

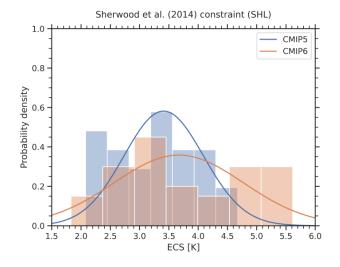


Fig. 32: Probability densities for the constrained ECS (solid lines) and the unconstrained model ensembles (histograms) of the emergent relationship shown in the figure above.

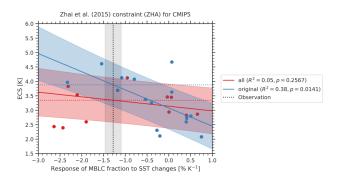


Fig. 33: Emergent relationship of the Zhai et al. (2015) emergent constraint for different subsets of CMIP5 models. Blue circles show the 15 CMIP5 models used in the original publication (except for CESM1-CAM5); the solid blue line and blue shaded area show the emergent relationships evaluated on these models including the uncertainty range. In this study, 11 more CMIP5 models have been added (red circles). The corresponding emergent relationship that considers all available CMIP5 models is shown in red colors. This relationship shows a considerably lower coefficient of determination ( $R^2$ ) and higher *p*-value than the relationship using the original subset of CMIP5 models. The vertical dashed line and shaded area correspond to the observational reference, and the horizontal dashed lines show the corresponding ECS constraints using this observation.

# 17.8 Emergent constraint on equilibrium climate sensitivity from global temperature variability

#### 17.8.1 Overview

This recipe reproduces the emergent constraint proposed by Cox et al. (2018) for the equilibrium climate sensitivity (ECS) using global temperature variability. The latter is defined by a metric which can be calculated from the global temperature variance (in time)  $\sigma_T$  and the one-year-lag autocorrelation of the global temperature  $\alpha_{1T}$  by

$$\psi = \frac{\sigma_T}{\sqrt{-\ln(\alpha_{1T})}}$$

Using the simple Hasselmann model they show that this quantity is linearly correlated with the ECS. Since it only depends on the temporal evolution of the global surface temperature, there is lots of observational data available which allows the construction of an emergent relationship. This method predicts an ECS range of 2.2K to 3.4K (66% confidence limit).

#### 17.8.2 Available recipes and diagnostics

Recipes are stored in recipes/

• recipe\_cox18nature.yml

Diagnostics are stored in diag\_scripts/

- emergent\_constraints/cox18nature.py
- climate\_metrics/ecs.py
- climate\_metrics/psi.py

#### 17.8.3 User settings in recipe

- Preprocessor
  - area\_statistics (operation: mean): Calculate global mean.
- Script emergent\_constraints/cox18nature.py

See *here*.

Script climate\_metrics/ecs.py

See *here*.

- Script climate\_metrics/psi.py
  - output\_attributes, *dict*, optional: Write additional attributes to all output netcdf files.
  - lag, int, optional (default: 1): Lag (in years) for the autocorrelation function.
  - window\_length, int, optional (default: 55): Number of years used for the moving window average.

#### 17.8.4 Variables

- *tas* (atmos, monthly, longitude, latitude, time)
- tasa (atmos, monthly, longitude, latitude, time)

#### 17.8.5 Observations and reformat scripts

• HadCRUT4 (tasa)

#### 17.8.6 References

• Cox, Peter M., Chris Huntingford, and Mark S. Williamson. "Emergent constraint on equilibrium climate sensitivity from global temperature variability." Nature 553.7688 (2018): 319.

#### 17.8.7 Example plots

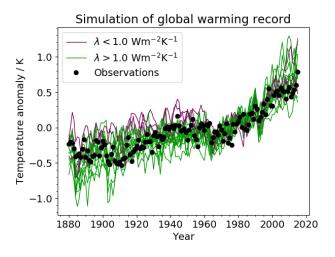


Fig. 34: Simulated change in global temperature from CMIP5 models (coloured lines), compared to the global temperature anomaly from the HadCRUT4 dataset (black dots). The anomalies are relative to a baseline period of 1961–1990. The model lines are colour-coded, with lower-sensitivity models ( > 1  $\text{Wm}^{-2}\text{K}^{-1}$ ) shown by green lines and highersensitivity models ( < 1  $\text{Wm}^{-2}\text{K}^{-1}$ ) shown by magenta lines.

## 17.9 Emergent constraint on snow-albedo effect

#### 17.9.1 Overview

The recipe recipe\_snowalbedo.yml computes the springtime snow-albedo feedback values in climate change versus springtime values in the seasonal cycle in transient climate change experiments following Hall and Qu (2006). The strength of the snow-albedo effect is quantified by the variation in net incoming shortwave radiation (Q) with surface air temperature ( $T_s$ ) due to changes in surface albedo  $\alpha_s$ :

$$\left(\frac{\partial Q}{\partial T_s}\right) = -I_t \cdot \frac{\partial \alpha_p}{\partial \alpha_s} \cdot \frac{\Delta \alpha_s}{\Delta T_s}$$

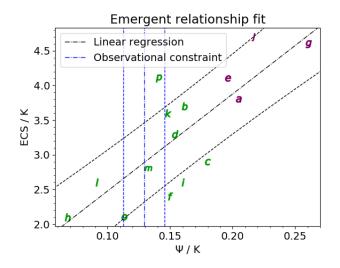


Fig. 35: Emergent relationship between ECS and the metric. The black dot-dashed line shows the best-fit linear regression across the model ensemble, with the prediction error for the fit given by the black dashed lines. The vertical blue lines show the observational constraint from the HadCRUT4 observations: the mean (dot-dashed line) and the mean plus and minus one standard deviation (dashed lines).

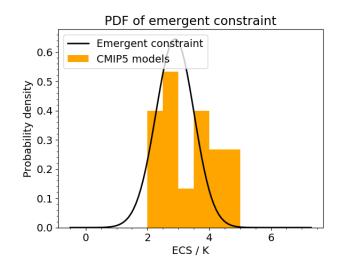


Fig. 36: The PDF for ECS. The orange histograms (both panels) show the prior distributions that arise from equal weighting of the CMIP5 models in 0.5 K bins.

The diagnostic produces scatterplots of simulated springtime  $\Delta \alpha_s / \Delta T_s$  values in climate change (ordinate) vs. simulated springtime  $\Delta \alpha_s / \Delta T_s$  values in the seasonal cycle (abscissa).

Ordinate values: the change in April  $\alpha_s$  (future projection - historical) averaged over NH land masses poleward of 30°N is divided by the change in April T<sub>s</sub> (future projection - historical) averaged over the same region. The change in  $\alpha_s$  (or T<sub>s</sub>) is defined as the difference between 22nd-century-mean  $\alpha_s$ : (T<sub>s</sub>) and 20th-century-mean  $\alpha_s$ . Values of  $\alpha_s$  are weighted by April incoming insolation (I<sub>t</sub>) prior to averaging.

Abscissa values: the seasonal cycle  $\Delta \alpha_s / \Delta T_s$  values, based on 20th century climatological means, are calculated by dividing the difference between April and May  $\alpha_s$ : averaged over NH continents poleward of 30°N by the difference between April and May  $T_s$  averaged over the same area. Values of  $\alpha_s$ : are weighted by April incoming insolation prior to averaging.

## 17.9.2 Available recipes and diagnostics

Recipes are stored in recipes/

• recipe\_snowalbedo.yml

Diagnostics are stored in diag\_scripts/emergent\_constraints/

• snowalbedo.ncl: springtime snow-albedo feedback values vs. seasonal cycle

## 17.9.3 User settings in recipe

1. Script snowalbedo.ncl

Required settings for script

- exp\_presentday: name of present-day experiment (e.g. "historical")
- exp\_future: name of climate change experiment (e.g. "rcp45")

#### Optional settings for script

- diagminmax: observational uncertainty (min and max)
- legend\_outside: create extra file with legend (true, false)
- styleset: e.g. "CMIP5" (if not set, this diagnostic will create its own color table and symbols for plotting)
- suffix: string to be added to output filenames
- xmax: upper limit of x-axis (default = automatic)
- xmin: lower limit of x-axis (default = automatic)
- ymax: upper limit of y-axis (default = automatic)
- ymin: lower limit of y-axis (default = automatic)

Required settings for variables

• ref\_model: name of reference data set

Optional settings for variables

none

```
Required settings (scripts)
```

none

Optional settings (scripts)

## 17.9.4 Variables

- tas (atmos, monthly mean, longitude latitude time)
- rsdt (atmos, monthly mean, longitude latitude time)
- rsuscs, rsdscs (atmos, monthly mean, longitude latitude time)

## 17.9.5 Observations and reformat scripts

- ERA-Interim (tas esmvaltool/cmorizers/data/formatters/datasets/era\_interim.py)
- ISCCP-FH (rsuscs, rsdscs, rsdt esmvaltool/cmorizers/data/formatters/datasets/isccp\_fh.ncl)

## 17.9.6 References

- Flato, G., J. Marotzke, B. Abiodun, P. Braconnot, S.C. Chou, W. Collins, P. Cox, F. Driouech, S. Emori, V. Eyring, C. Forest, P. Gleckler, E. Guilyardi, C. Jakob, V. Kattsov, C. Reason and M. Rummukainen, 2013: Evaluation of Climate Models. In: Climate Change 2013: The Physical Science Basis. Contribution of Working Group I to the Fifth Assessment Report of the Intergovernmental Panel on Climate Change [Stocker, T.F., D. Qin, G.-K. Plattner, M. Tignor, S.K. Allen, J. Boschung, A. Nauels, Y. Xia, V. Bex and P.M. Midgley (eds.)]. Cambridge University Press, Cambridge, United Kingdom and New York, NY, USA.
- Hall, A., and X. Qu, 2006: Using the current seasonal cycle to constrain snow albedo feedback in future climate change, Geophys. Res. Lett., 33, L03502, doi:10.1029/2005GL025127.

## 17.9.7 Example plots

## 17.10 Equilibrium climate sensitivity

#### 17.10.1 Overview

Equilibrium climate sensitivity is defined as the change in global mean temperature as a result of a doubling of the atmospheric  $CO_2$  concentration compared to pre-industrial times after the climate system has reached a new equilibrium. This recipe uses a regression method based on Gregory et al. (2004) to calculate it for several CMIP models.

## 17.10.2 Available recipes and diagnostics

Recipes are stored in recipes/

• recipe\_ecs.yml

Diagnostics are stored in diag\_scripts/

- climate\_metrics/ecs.py
- climate\_metrics/create\_barplot.py
- climate\_metrics/create\_scatterplot.py

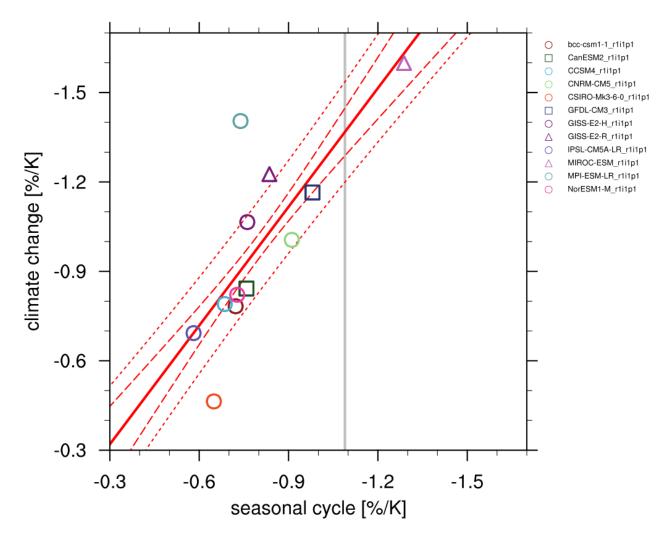


Fig. 37: Scatterplot of springtime snow-albedo effect values in climate change vs. springtime  $\Delta \alpha_s / \Delta T_s$  values in the seasonal cycle in transient climate change experiments (CMIP5 historical experiments: 1901-2000, RCP4.5 experiments: 2101-2200). Similar to IPCC AR5 Chapter 9 (Flato et al., 2013), Figure 9.45a.

## 17.10.3 User settings in recipe

- Preprocessor
  - area\_statistics (*operation: mean*): Calculate global mean.
- Script climate\_metrics/ecs.py
  - calculate\_mmm, bool, optional (default: True): Calculate multi-model mean ECS.
  - complex\_gregory\_plot, *bool*, optional (default: False): Plot complex Gregory plot (also add response for first sep\_year years and last 150 - sep\_year years, default: sep\_year=20) if True.
  - output\_attributes, *dict*, optional: Write additional attributes to netcdf files.
  - read\_external\_file, *str*, optional: Read ECS and feedback parameters from external file. The path can be given relative to this diagnostic script or as absolute path.
  - savefig\_kwargs, *dict*, optional: Keyword arguments for matplotlib.pyplot.savefig().
  - seaborn\_settings, *dict*, optional: Options for seaborn.set\_theme() (affects all plots).
  - sep\_year, *int*, optional (default: 20): Year to separate regressions of complex Gregory plot. Only effective if complex\_gregory\_plot is True.
  - x\_lim, list of float, optional (default: [1.5, 6.0]): Plot limits for X axis of Gregory regression plot (T).
  - y\_lim, *list of float*, optional (default: [0.5, 3.5]): Plot limits for Y axis of Gregory regression plot (N).
- Script climate\_metrics/create\_barplot.py
  - add\_mean, str, optional: Add a bar representing the mean for each class.
  - label\_attribute, str, optional: Cube attribute which is used as label for different input files.
  - order, *list of str*, optional: Specify the order of the different classes in the barplot by giving the label, makes most sense when combined with label\_attribute.
  - patterns, *list of str*, optional: Patterns to filter list of input data.
  - savefig\_kwargs, *dict*, optional: Keyword arguments for matplotlib.pyplot.savefig().
  - seaborn\_settings, *dict*, optional: Options for seaborn.set\_theme() (affects all plots).
  - sort\_ascending, bool, optional (default: False): Sort bars in ascending order.
  - sort\_descending, *bool*, optional (default: False): Sort bars in descending order.
  - subplots\_kwargs, *dict*, optional: Keyword arguments for matplotlib.pyplot.subplots().
  - value\_labels, *bool*, optional (default: False): Label bars with value of that bar.
  - y\_range, *list of float*, optional: Range for the Y axis of the plot.
- Script climate\_metrics/create\_scatterplot.py
  - dataset\_style, *str*, optional: Name of the style file (located in esmvaltool.diag\_scripts.shared. plot.styles\_python).
  - pattern, *str*, optional: Pattern to filter list of input files.
  - seaborn\_settings, *dict*, optional: Options for seaborn.set\_theme() (affects all plots).
  - y\_range, *list of float*, optional: Range for the Y axis of the plot.

## 17.10.4 Variables

- *rlut* (atmos, monthly, longitude, latitude, time)
- *rsdt* (atmos, monthly, longitude, latitude, time)
- rsut (atmos, monthly, longitude, latitude, time)
- tas (atmos, monthly, longitude, latitude, time)

## 17.10.5 Observations and reformat scripts

#### None

#### 17.10.6 References

• Gregory, Jonathan M., et al. "A new method for diagnosing radiative forcing and climate sensitivity." Geophysical research letters 31.3 (2004).

## 17.10.7 Example plots

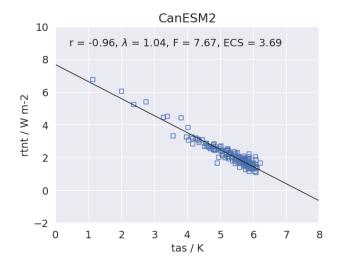


Fig. 38: Scatterplot between TOA radiance and global mean surface temperature anomaly for 150 years of the abrupt 4x CO2 experiment including linear regression to calculate ECS for CanESM2 (CMIP5).

## 17.11 KNMI Climate Scenarios 2014

#### 17.11.1 Overview

This recipe implements the method described in Lenderink et al., 2014, to prepare the 2014 KNMI Climate Scenarios (KCS) for the Netherlands. A set of 8 global climate projections from EC-Earth were downscaled with the RACMO regional climate model. Since the EC-Earth ensemble is not readily representative for the spread in the full CMIP ensemble, this method recombines 5-year segments from the EC-Earth ensemble to obtain a large suite of "resamples". Subsequently, 8 new resamples are selected that cover the spread in CMIP much better than the original set.

The original method created 8 resampled datasets:

- 2 main scenarios: Moderate (M) and Warm (W) (Lenderink 2014 uses "G" instead of "M").
- 2 'sub'scenarios: Relatively high (H) or low (L) changes in seasonal temperature and precipitation
- 2 time horizons: Mid-century (MOC; 2050) and end-of-century (EOC; 2085)
- Each scenario consists of changes calculated between 2 periods: Control (e.g. 1981-2010) and future (variable).

The configuration settings for these resamples can be found in table 1 of Lenderink 2014's supplementary data.

## 17.11.2 Implementation

The implementation is such that application to other datasets, regions, etc. is relatively straightforward. The description below focuses on the reference use case of Lenderink et al., 2014, where the target model was EC-Earth. An external set of EC-Earth data (all RCP85) was used, for which 3D fields for downscaling were available as well. In the recipe shipped with ESMValTool, however, the target model is CCSM4, so that it works out of the box with ESGF data only.

In the first diagnostic, the spread of the full CMIP ensemble is used to obtain 4 values of a *global*  $\Delta T_{CMIP}$ , corresponding to the 10th and 90th percentiles for the M and W scenarios, respectively, for both MOC and EOC. Subsequently, for each of these 4 *steering parameters*, 30-year periods are selected from the target model ensemble, where  $\Delta T_{target} \approx \Delta T_{CMIP}$ .

In the second diagnostic, for both the control and future periods, the N target model ensemble members are split into 6 segments of 5 years each. Out of all  $N^6$  possible re-combinations of these 5-year segments, eventually M new 'resamples' are selected based on *local* changes in seasonal temperature and precipitation. This is done in the following steps:

- 1. Select 1000 samples for the control period, and 2 x 1000 samples for the future period (one for each subscenario). Step 1 poses a constraint on winter precipitation. For the control period, winter precipitation must still closely represent the average of the original ensemble. For the two future periods, the change in winter precipitation with respect to the control period must approximately equal 4% per degree  $\Delta T$  (subscenario L) or 8% per degree  $\Delta T$  (subscenario H).
- 2. Further constrain the selection by picking samples that represent either high or low changes in summer precipitation and summer and winter temperature, by limiting the remaining samples to certain percentile ranges: relatively wet/cold in the control and dry/warm in the future, or vice versa. The percentile ranges are listed in table 1 of Lenderink 2014's supplement. This should result is approximately 50 remaining samples for each scenario, for both control and future.
- 3. Use a Monte-Carlo method to make a final selection of 8 resamples with minimal reuse of the same ensemble member/segment.

Datasets have been split in two parts: the CMIP datasets and the target model datasets. An example use case for this recipe is to compare between CMIP5 and CMIP6, for example. The recipe can work with a target model that is not part of CMIP, provided that the data are CMOR compatible, and using the same data referece syntax as the CMIP data. Note that you can specify multiple data paths in the user configuration file.

#### 17.11.3 Available recipes and diagnostics

Recipes are stored in recipes/

• recipe\_kcs.yml

Diagnostics are stored in diag\_scripts/kcs/

- global\_matching.py
- local\_resampling.py

**Note:** We highly recommend using the options described in *Re-running diagnostics*. The speed bottleneck for the first diagnostic is the preprocessor. In the second diagnostic, step 1 is most time consuming, whereas steps 2 and 3 are likely to be repeated several times. Therefore, intermediate files are saved after step 1, and the diagnostic will automatically detect and use them if the -i flag is used.

## 17.11.4 User settings

1. Script <global\_matching.py>

Required settings for script

- scenario\_years: a list of time horizons. Default: [2050, 2085]
- scenario\_percentiles: a list of percentiles for the steering table. Default: [p10, p90]

*Required settings for preprocessor* This diagnostic needs global mean temperature anomalies for each dataset, both CMIP and the target model. Additionally, the multimodel statistics preprocessor must be used to produce the percentiles specified in the setting for the script above.

2. Script <local\_resampling.py>

Required settings for script

- control\_period: the control period shared between all scenarios. Default: [1981, 2010]
- n\_samples: the final number of recombinations to be selected. Default: 8
- scenarios: a scenario name and list of options. The default setting is a single scenario:

```
scenarios:
ML_MOC: # scenario name; can be chosen by the user
description: "Moderate / low changes in seasonal temperature &_
oprecipitation"
global_dT: 1.0
scenario_year: 2050
resampling_period: [2021, 2050]
dpr_winter: 4
pr_summer_control: [25, 55]
pr_summer_future: [45, 75]
tas_winter_control: [50, 80]
tas_winter_future: [20, 50]
tas_summer_control: [0, 100]
tas_summer_future: [0, 50]
```

These values are taken from table 1 in the Lenderink 2014's supplementary material. Multiple scenarios can be processed at once by appending more configurations below the default one. For new applications, global\_dT, resampling\_period and dpr\_winter are informed by the output of the first diagnostic. The percentile bounds in the scenario settings (e.g. tas\_winter\_control and tas\_winter\_future) are to be tuned until a satisfactory scenario spread over the full CMIP ensemble is achieved.

#### Required settings for preprocessor

This diagnostic requires data on a single point. However, the extract\_point preprocessor can be changed to extract\_shape or extract\_region, in conjunction with an area mean. And of course, the coordinates can be changed to analyze a different region.

#### 17.11.5 Variables

Variables are precipitation and temperature, specified separately for the target model and the CMIP ensemble:

- pr\_target (atmos, monthly mean, longitude latitude time)
- tas\_target (atmos, monthly mean, longitude latitude time)
- pr\_cmip (atmos, monthly mean, longitude latitude time)
- tas\_cmip (atmos, monthly mean, longitude latitude time)

#### 17.11.6 References

• Lenderink et al. 2014, Environ. Res. Lett., 9, 115008.

#### 17.11.7 Example output

The diagnostic global\_matching produces a scenarios table like the one below

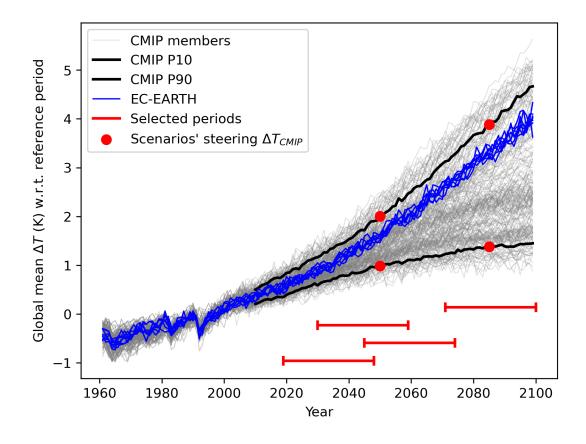
yea	r percentile cm	ip_dt	period_bounds	target_dt	<pre>pattern_scaling_factor</pre>
0 205	0 P10	0.98	[2019, 2048]	0.99	1.00
1 205	0 P90	2.01	[2045, 2074]	2.02	0.99
2 208	5 P10	1.38	[2030, 2059]	1.38	1.00
3 208	5 P90	3.89	[2071, 2100]	3.28	1.18

which is printed to the log file and also saved as a csv-file scenarios.csv. Additionally, a figure is created showing the CMIP spread in global temperature change, AND highlighting the selected steering parameters and resampling periods:

The diagnostic local\_resampling procudes a number of output files:

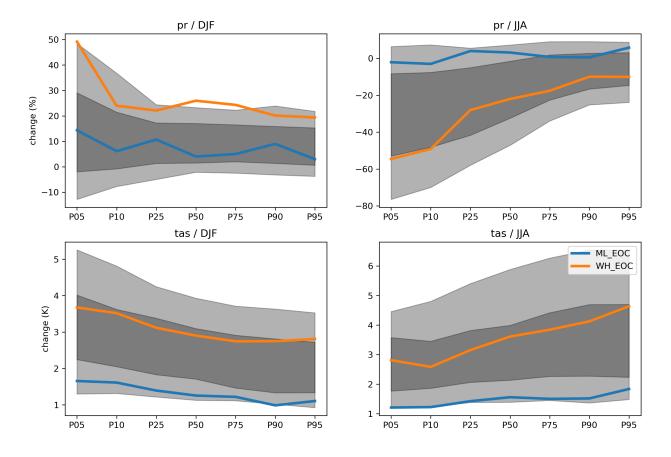
- season\_means\_<scenario>.nc: intermediate results, containing the season means for each segment of the original target model ensemble.
- top1000\_<scenario>.csv: intermediate results, containing the 1000 combinations that have been selected based on winter mean precipitation.
- indices\_<scenario>.csv: showing the final set of resamples as a table:

	cont: Segment		t 1 Segment	2 Segment	t 3 Segment	4 Segment		ure t
→ <b>0</b> Segment	1 Segment	2 Segment	3 Segment	4 Segment	5			
Combination	0	5	7	6	3	1	3	<b>.</b>
<u></u> →2	4	2	4	7	7			
						(coi	ntinues on next	page)



						(con	tinued from pre	vious page)
Combination	1	0	3	0	4	3	2	
-→4	1	6	1	3	0			
Combination	2	2	4	3	7	4	2	
<b>⇔</b> 5	4	6	6	4	2			
Combination	3	1	4	7	2	3	6	<b>_</b>
<b>⇔</b> 5	3	1	7	4	1			
Combination	4	5	7	6	3	1	3	
⇔2	3	0	6	1	7			
Combination	5	7	2	1	4	5	1	
<b>⇔</b> 6	0	4	2	3	3			
Combination	6	7	2	2	0	6	6	
⊶ <b>5</b>	2	1	5	4	2			
Combination	7	6	3	2	1	6	1	
⇔2	1	0	2	1	3			

- resampled\_control\_<scenario>.nc: containing the monthly means for the control period according to the final combinations.
- resampled\_future\_<scenario>.nc: containing the monthly means for the future period according to the final combinations.
- Provenance information: bibtex, xml, and/or text files containing citation information are stored alongside the final result and the final figure. The final combinations only derive from the target model data, whereas the figure also uses CMIP data.
- A figure used to validate the final result, reproducing figures 5 and 6 from Lenderink et al.:



Year: 2085

## 17.12 Multiple ensemble diagnostic regression (MDER) for constraining future austral jet position

## 17.12.1 Overview

Wenzel et al. (2016) use multiple ensemble diagnostic regression (MDER) to constrain the CMIP5 future projection of the summer austral jet position with several historical process-oriented diagnostics and respective observations.

The following plots are reproduced:

- Absolute correlation between the target variable and the diagnostics.
- Scatterplot between the target variable and the MDER-calculated linear combination of diagnostics.
- Boxplot of RMSE for the unweighted multi-model mean and the (MDER) weighted multi-model mean of the target variable in a pseudo-reality setup.
- Time series of the target variable for all models, observations and MDER predictions.
- Errorbar plots for all diagnostics.
- Scatterplots between the target variable and all diagnostics.

## 17.12.2 Available recipes and diagnostics

Recipes are stored in recipes/

• recipe\_wenzel16jclim.yml

Diagnostics are stored in diag\_scripts/

- austral\_jet/asr.ncl
- austral\_jet/main.ncl
- mder/absolute\_correlation.ncl
- mder/regression\_stepwise.ncl
- mder/select\_for\_mder.ncl

## 17.12.3 User settings in recipe

- 1. Preprocessor
  - extract\_region: Region extraction.
  - extract\_levels: Pressure level extraction.
  - area\_statistics: Spatial average calculations.
- 2. Script austral\_jet/asr.ncl
  - season, *str*: Season.
  - average\_ens, *bool*, optional (default: False): Average over all given ensemble members of a climate model.
  - wdiag, *array of str*, optional: Names of the diagnostic for MDER output. Necessary when MDER output is desired.
  - wdiag\_title, *array of str*, optional: Names of the diagnostic in plots.

- 3. Script austral\_jet/main.ncl
  - styleset, *str*: Style set used for plotting the multi-model plots.
  - season, *str*: Season.
  - average\_ens, *bool*, optional (default: False): Average over all given ensemble members of a climate model.
  - rsondes, array of str, optional: Additional observations used in the plot but not for MDER output.
  - rsondes\_file, *array of str*, optional: Paths to the additional observations Necessary when rsondes is given.
  - rsondes\_yr\_min, *int*, optional: Minimum year for additional observations. Necessary when rsondes is given.
  - rsondes\_yr\_max, *int*, optional: Maximum year for additional observations. Necessary when rsondes is given.
  - wdiag, *array of str*, optional: Names of the diagnostic for MDER output. Necessary when MDER output is desired.
  - wdiag\_title, array of str, optional: Names of the diagnostic in plots.
  - derive\_var, str, optional: Derive variables using NCL functions. Must be one of "tpp", "mmstf".
  - derive\_latrange, *array of float*, optional: Latitude range for variable derivation. Necessary if derive\_var is given.
  - derive\_lev, *float*, optional: Pressure level (given in *Pa*) for variable derivation. Necessary if derive\_var is given.
- 4. Script mder/absolute\_correlation.ncl
  - p\_time, array of int: Start years for future projections.
  - p\_step, *int*: Time range for future projections (in years).
  - scal\_time, *array of int*: Time range for base period (in years) for anomaly calculations used when calc\_type = "trend".
  - time\_oper, str: Operation used in NCL time\_operation function.
  - time\_opt, *str*: Option used in NCL time\_operation function.
  - calc\_type, str: Calculation type for the target variable. Must be one of "trend", "pos", "int".
  - domain, str: Domain tag for provenance tracking.
  - average\_ens, *bool*, optional (default: False): Average over all given ensemble members of a climate model.
  - region, *str*, optional: Region used for area aggregation. Necessary if input of target variable is multidimensional.
  - area\_oper, *str*, optional: Operation used in NCL area\_operation function. Necessary if multidimensional is given.
  - plot\_units, str, optional (attribute for variable\_info): Units for the target variable used in the plots.
- 5. Script mder/regression\_stepwise.ncl
  - p\_time, array of int: Start years for future projections.
  - p\_step, *int*: Time range for future projections (in years).

- scal\_time, *array of int*: Time range for base period (in years) for anomaly calculations used when calc\_type = "trend".
- time\_oper, *str*: Operation used in NCL time\_operation function.
- time\_opt, *str*: Option used in NCL time\_operation function.
- calc\_type, str: Calculation type for the target variable. Must be one of "trend", "pos", "int".
- domain, *str*: Domain tag for provenance tracking.
- average\_ens, *bool*, optional (default: False): Average over all given ensemble members of a climate model.
- smooth, bool, optional (default: False): Smooth time period with 1-2-1 filter.
- iter, int, optional: Number of iterations for smoothing. Necessary when smooth is given.
- cross\_validation\_mode, bool, optional (default: False): Perform cross-validation.
- region, *str*, optional: Region used for area aggregation. Necessary if input of target variable is multidimensional.
- area\_oper, *str*, optional: Operation used in NCL area\_operation function. Necessary if multidimensional is given.
- plot\_units, *str*, optional (attribute for variable\_info): Units for the target variable used in the plots.
- 6. Script mder/select\_for\_mder.ncl
  - wdiag, array of str: Names of the diagnostic for MDER output. Necessary when MDER output is desired.
  - domain, *str*: Domain tag for provenance tracking.
  - ref\_dataset, *str*: Style set used for plotting the multi-model plots.
  - average\_ens, *bool*, optional (default: False): Average over all given ensemble members of a climate model.
  - derive\_var, str, optional: Derive variables using NCL functions. Must be one of "tpp", "mmstf".

## 17.12.4 Variables

- *ta* (atmos, monthly, longitude, latitude, pressure level, time)
- *uajet* (atmos, monthly, time)
- va (atmos, monthly, longitude, latitude, pressure level, time)
- *ps* (atmos, monthly, longitude, latitude, time)
- asr (atmos, monthly, longitude, latitude, time)

#### 17.12.5 Observations and reformat scripts

- ERA-Intermin (ta, uajet, va, ps)
- CERES-EBAF (asr)

#### 17.12.6 References

• Wenzel, S., V. Eyring, E.P. Gerber, and A.Y. Karpechko: Constraining Future Summer Austral Jet Stream Positions in the CMIP5 Ensemble by Process-Oriented Multiple Diagnostic Regression. J. Climate, 29, 673–687, doi:10.1175/JCLI-D-15-0412.1, 2016.

#### 17.12.7 Example plots

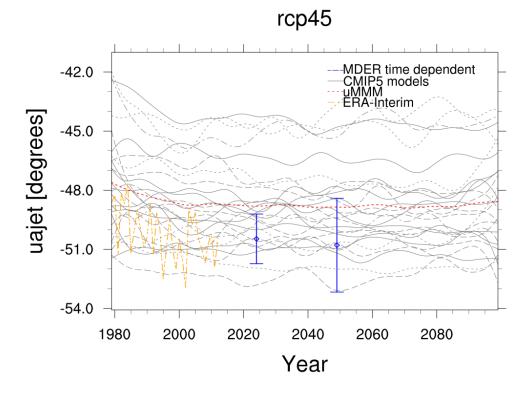


Fig. 39: Time series of the the target variable (future austral jet position in the RCP 4.5 scenario) for the CMIP5 ensemble, observations, unweighted multi-model mean projections and (MDER) weighted multi-model mean projections.

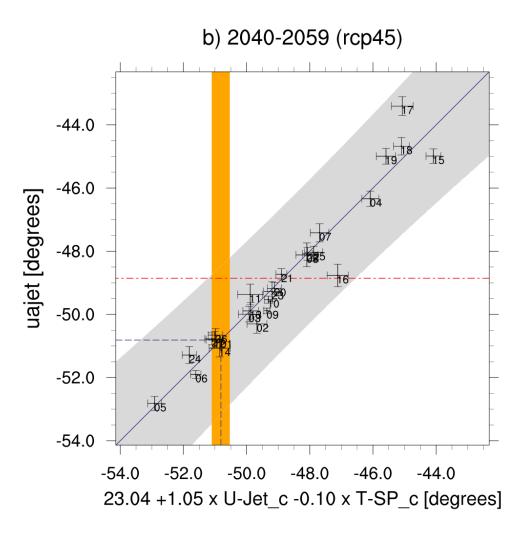


Fig. 40: Scatterplot of the target variable (future austral jet position in the RCP 4.5 scenario) vs. the MDER-determined linear combination of diagnostics for the CMIP5 ensemble.

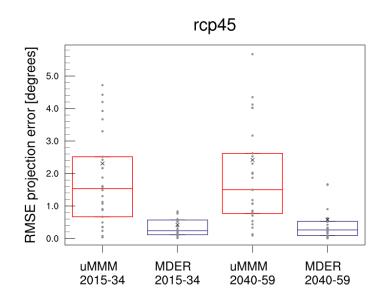


Fig. 41: Boxplot for the RMSE of the target variable for the unweighted and (MDER) weighted multi-model mean projections in a pseudo-reality setup.

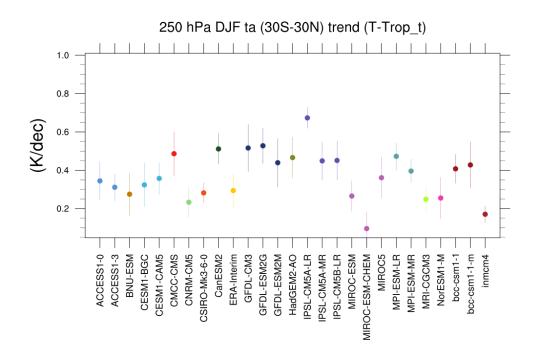


Fig. 42: Trends in tropical DJF temperature at 250hPa for different CMIP5 models and observations.

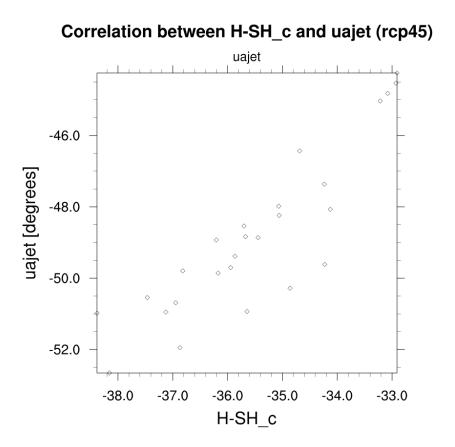


Fig. 43: Scatterplot of the target variable (future austral jet position in the RCP 4.5 scenario) vs. a single diagnostic, the historical location of the Southern hemisphere Hadley cell boundary for the CMIP5 ensemble.

# 17.13 Projected land photosynthesis constrained by changes in the seasonal cycle of atmospheric CO<sub>2</sub>

## 17.13.1 Overview

Selected figures from Wenzel et al. (2016) are reproduced with recipe\_wenzel16nat.yml. Gross primary productivity (gpp) and atmospheric CO<sub>2</sub> concentrations at the surface (co2s) are analyzed for the carbon cycle - concentration feedback in the historical (esmHistorical) and uncoupled (esmFixCLim1, here the carbon cycle is uncoupled to the climate response) simulations. The recipe includes a set of routines to diagnose the long-term carbon cycle - concentration feedback parameter (beta) from an ensemble of CMIP5 models and the observable change in the CO<sub>2</sub> seasonal cycle amplitude due to rising atmospheric CO<sub>2</sub> levels. As a key figure of this recipe, the diagnosed values from the models beta vs. the change in CO<sub>2</sub> amplitude are compared in a scatter plot constituting an emergent constraint.

## 17.13.2 Available recipe and diagnostics

Recipes are stored in recipes/

• recipe\_wenzel16nat.yml

Diagnostics are stored in diag\_scripts/carbon\_ec/

- carbon\_beta: (1) scatter plot of annual gpp vs. annual  $CO_2$  and (2) barchart of  $gpp(2xCO_2)/gpp(1xCO_2)$ ; calculates beta for emergent constraint (carbon\_co2\_cycle.ncl)
- carbon\_co2\_cycle.ncl: (1) scatter plot of CO<sub>2</sub> amplitude vs. annual CO<sub>2</sub>, (2) barchart of sensitivity of CO<sub>2</sub> amplitude to CO<sub>2</sub>, (3) emergent constraint: gpp(2xCO<sub>2</sub>)/gpp(1xCO<sub>2</sub>) vs. sensitivity of CO<sub>2</sub> amplitude to CO<sub>2</sub>, (4) probability density function of constrained and unconstrained sensitivity of CO<sub>2</sub> amplitude to CO<sub>2</sub>

## 17.13.3 User settings

**Note:** Make sure to run this recipe setting output\_file\_type: pdf in the config\_user.yml file or using the CLI flag --output\_file\_type=pdf.

1. Script carbon\_beta.ncl

Required Settings (scripts)

• styleset: project style for lines, colors and symbols

**Optional Settings (scripts)** 

- bc\_xmax\_year: end year to calculate beta (default: use last available year of all models)
- bc\_xmin\_year: start year to calculate beta (default: use first available year of all models)

Required settings (variables)

none

Optional settings (variables)

none

2. Script carbon\_co2\_cycle.ncl

Required Settings (scripts)

- nc\_infile: path of netCDF file containing beta (output from carbon\_beta.ncl)
- styleset: project style for lines, colors and symbols

**Optional Settings (scripts)** 

- bc\_xmax\_year: end year (default = last year of all model datasets available)
- bc\_xmin\_year: start year (default = first year of all model datasets available)

Required settings (variables)

• reference\_dataset: name of reference dataset (observations)

Optional settings (variables)

none

### 17.13.4 Variables

- co2s (atmos, monthly mean, plev longitude latitude time)
- gpp (land, monthly mean, longitude latitude time)

### 17.13.5 Observations and reformat scripts

• ESRL: Earth System Research Laboratory, ground-based CO<sub>2</sub> measurements

### 17.13.6 References

• Wenzel, S., Cox, P., Eyring, V. et al., 2016, Projected land photosynthesis constrained by changes in the seasonal cycle of atmospheric CO<sub>2</sub>. Nature 538, 499501, doi: doi.org/10.1038/nature19772

## 17.13.7 Example plots

# **17.14 Transient Climate Response**

### 17.14.1 Overview

The transient climate response (TCR) is defined as the global and annual mean surface air temperature anomaly in the *lpctCO2* scenario (1% CO<sub>2</sub> increase per year) for a 20 year period centered at the time of CO<sub>2</sub> doubling, i.e. using the years 61 to 80 after the start of the simulation. We calculate the temperature anomaly by subtracting a linear fit of the *piControl* run for all 140 years of the *lpctCO2* experiment prior to the TCR calculation (see Gregory and Forster, 2008).

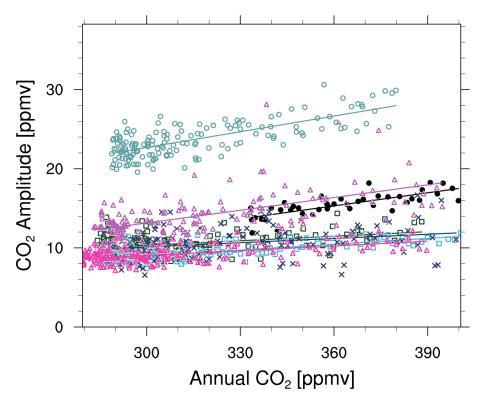


Fig. 44: Comparison of  $CO_2$  seasonal amplitudes for CMIP5 historical simulations and observations showing annual mean atmospheric  $CO_2$  versus the amplitudes of the  $CO_2$  seasonal cycle at Pt. Barrow, Alaska (produced with carbon\_co2\_cycle.ncl, similar to Fig. 1a from Wenzel et al. (2016)).

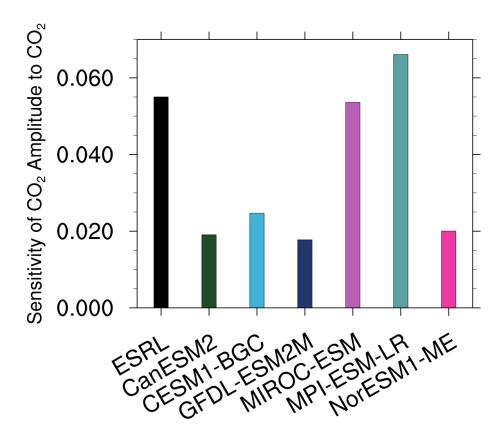


Fig. 45: Barchart showing the gradient of the linear correlations for the comparison of  $CO_2$  seasonal amplitudes for CMIP5 historical for at Pt. Barrow, Alaska (produced with carbon\_co2\_cycle.ncl, similar to Fig. 1b from Wenzel et al. (2016)).

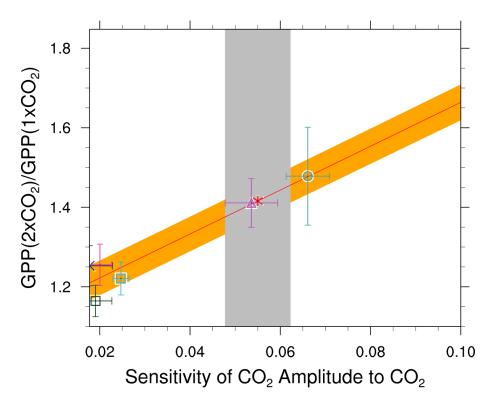


Fig. 46: Emergent constraint on the relative increase of large-scale GPP for a doubling of  $CO_2$ , showing the correlations between the sensitivity of the  $CO_2$  amplitude to annual mean  $CO_2$  increases at Pt. Barrow (x-axis) and the high-latitude (60N - 90N)  $CO_2$  fertilization on GPP at  $2xCO_2$ . The red line shows the linear best fit of the regression together with the prediction error (orange shading), the gray shading shows the observed range (produced with carbon\_co2\_cycle.ncl, similar to Fig. 3a from Wenzel et al. (2016)).

### 17.14.2 Available recipes and diagnostics

Recipes are stored in recipes/

• recipe\_tcr.yml

Diagnostics are stored in diag\_scripts/

- climate\_metrics/tcr.py
- climate\_metrics/create\_barplot.py
- climate\_metrics/create\_scatterplot.py

## 17.14.3 User settings in recipe

- Preprocessor
  - area\_statistics (*operation: mean*): Calculate global mean.
- Script climate\_metrics/tcr.py
  - calculate\_mmm, *bool*, optional (default: True): Calculate multi-model mean TCR.
  - plot, *bool*, optional (default: True): Plot temperature vs. time.
  - read\_external\_file, *str*, optional: Read TCR from external file. The path can be given relative to this diagnostic script or as absolute path.
  - savefig\_kwargs, *dict*, optional: Keyword arguments for matplotlib.pyplot.savefig().
  - seaborn\_settings, *dict*, optional: Options for seaborn.set\_theme() (affects all plots).
- Script climate\_metrics/create\_barplot.py

See *here*.

• Script climate\_metrics/create\_scatterplot.py

See *here*.

### 17.14.4 Variables

• tas (atmos, monthly, longitude, latitude, time)

## 17.14.5 Observations and reformat scripts

#### None

### 17.14.6 References

• Gregory, J. M., and P. M. Forster. "Transient climate response estimated from radiative forcing and observed temperature change." Journal of Geophysical Research: Atmospheres 113.D23 (2008).

## 17.14.7 Example plots

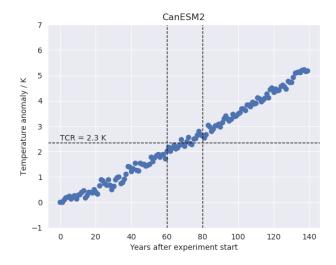


Fig. 47: Time series of the global mean surface air temperature anomaly (relative to the linear fit of the pre-industrial control run) of CanESM2 (CMIP5) for the 1% CO<sub>2</sub> increase per year experiment. The horizontal dashed line indicates the transient climate response (TCR) defined as the 20 year average temperature anomaly centered at the time of CO<sub>2</sub> doubling (vertical dashed lines).

# 17.15 Climate model projections from the ScenarioMIP of CMIP6

### 17.15.1 Overview

This recipe is implemented into ESMValTool to evaluate the temperature and precipitation changes from the ScenarioMIP of CMIP6. It produces the original plots and tables of Tebaldi et al. (2021), https://doi.org/10.5194/esd-12-253-2021

## 17.15.2 Available recipe and diagnostics

Recipe is stored in esmvaltool/recipes/

• recipe\_tebaldi21esd.yml

Diagnostics are stored in esmvaltool/diag\_scripts/tebaldi21esd/

- calc\_timeseries\_across\_realization\_stddev\_runave.ncl: computes time series of ensemble spreads (i.e., intermember standard deviations). One dataset is used for resampling subsets of 10 members.
- calc\_cmip6\_and\_cmip5\_pattern\_diff\_scaleT.ncl: computes the pattern difference between the CMIP6 multi-model mean change and the CMIP5 multi-model mean change.
- calc\_IAV\_hatching.ncl: computes the interannual variability (IAV) over piControl runs, either over the whole time period or in chunks over some years.
- calc\_pattern\_diff\_scaleT.ncl: computes the map of multi-model mean change scaled by global T change.
- calc\_pattern\_stippling\_hatching.ncl: computes the map of multi-model mean change with stippling for significant region and hatching for non-significant region. Significant is where the multi-model mean change is greater than two standard deviations of the internal variability and where at least 90% of the models agree on the sign

of change. Not significant is where the multi-model mean change is less than one standard deviation of internal variability.

- calc\_pattern\_intermodel\_stddev\_scaleT.ncl: computes the intermodel standard deviation of the change scaled by global T change standard deviation of the change scaled by global T change
- calc\_pattern\_interscenario\_stddev\_scaleT.ncl: computes the interscenario standard deviation of the change scaled by global T change
- calc\_pattern\_stddev\_scaleT.ncl: computes the standard deviation of the change scaled by global T change
- calc\_pattern\_comparison.ncl: computes the difference between the patterns of multi-model mean change of two different scenarios (ex: SSP4-6.0 and SSP4-3.4)
- calc\_table\_changes.ncl: computes the changes (mean and spreads) for the specified scenarios and time periods relative to the historical baseline.
- calc\_table\_warming\_level.ncl: computes the warming level crossing year (mean, five percent and ninety-five percent quantiles of crossing years) for specified scenarios and warming levels.
- calc\_timeseries\_mean\_spread\_runave.ncl: computes multi-model time series of change against historical baseline for specified scenarios with spread. A running average with specified window is performed.
- calc\_timeseries\_mean\_spread\_ssp4.ncl: computes multi-model time series of change against historical baseline for specified ssp434 and ssp460 with spread. A running average with specified window is performed.
- calc\_timeseries\_mean\_spread\_ssp5.ncl: computes multi-model time series of change against historical baseline for ssp534-over and ssp585 with spread. A running average with specified window is performed.
- plot\_pattern.ncl: plots a pattern.
- plot\_table\_changes: plots a table of the multi-model mean and spread for specified scenarios and periods.
- plot\_table\_warming\_level.ncl: plots a table of warming level crossing years for specified scenarios (columns) and warming levels (rows).
- plot\_timeseries\_mean\_spread\_3scenarios.ncl: plots time series (multi- model mean and spread) for 3 scenarios.
- plot\_timeseries\_mean\_spread\_constrained\_projections.ncl: plot time series with brackets for constrained projections.
- plot\_timeseries\_mean\_spread.ncl: plot time series (multi-model mean and spread) for 5 scenarios.
- plot\_timeseries\_mean\_spread\_rightaxis\_5scen.ncl: plot time series (multi-model mean and spread) for 5 scenarios and with an additional right axis.
- plot\_timeseries\_mean\_spread\_ssp4.ncl: plot time series for two ssp4 scenarios.
- plot\_timeseries\_mean\_spread\_ssp5.ncl: plot time series for two ssp5 scenarios.
- plot\_timeseries\_across\_realization\_stddev\_runave.ncl: plot time series of inter-member standard deviation.

### 17.15.3 User settings in recipe

1. Script calc\_timeseries\_across\_realization\_stddev\_runave.ncl

Required settings for script

- scenarios: list with scenarios included in figure
- syears: list with start years in time periods (e.g. start of historical period and SSPs)
- eyears: list with end years in time periods (end year of historical runs and SSPs)
- begin\_ref\_year: start year of reference period (e.g. 1995)

- end\_ref\_year: end year of reference period (e.g. 2014)
- n\_samples: number of samples of size 10 to draw among all the ensembles of sampled\_model
- sampled\_model: name of dataset on which to sample
- runave\_window: size window used for the centered running average
- 2. Script calc\_cmip6\_and\_cmip5\_pattern\_diff\_scaleT.ncl

- scenarios\_cmip5: list of CMIP5 scenarios included in figure
- scenarios\_cmip6: list of CMIP6 scenarios included in figure
- periods: list with start years of periods to be included
- time\_avg: time\_avg: time averaging ("annualclim", "seasonalclim")

#### Optional settings for script

- percent: determines if difference expressed in percent (0, 1, default= 0)
- 3. Script calc\_IAV\_hatching.ncl

#### Required settings for script

• time\_avg: time\_avg: time averaging ("annualclim", "seasonalclim") needs to be consistent with calc\_pattern\_stippling\_hatching.ncl

Optional settings for script

- periodlength: length of period in years to calculate variability over, default is total time period
- iavmode: calculate IAV from multi-model mean or save individual models ("each": save individual models, "mmm": multi-model mean, default), needs to be consistent with calc\_pattern\_stippling\_hatching.ncl
- 4. Script calc\_pattern\_diff\_scaleT.ncl

Required settings for script

- scenarios: list with scenarios included in figure
- periods: list with start years of periods to be included
- time\_avg: time\_avg: time averaging ("annualclim", "seasonalclim")
- 5. Script calc\_pattern\_stippling\_hatching.ncl

#### Required settings for script

- ancestors: variable and diagnostics that calculated interannual variability for stiplling and hatching
- time\_avg: time\_avg: time averaging ("annualclim", "seasonalclim") needs to be consistent with calc\_IAV\_hatching.ncl
- scenarios: list with scenarios to be included
- periods: list with start years of periods to be included
- labels: list with labels to use in legend depending on scenarios
- sig: plot stippling for significance? (True, False)
- not\_sig: plot hatching for uncertainty? (True, False)

- seasons: list with season index if time\_avg is "seasonalclim" (then seasons is required), DJF:0, MAM:1, JJA:2, SON:3
- iavmode: calculate IAV from multi-model mean or save individual models ("each": save individual models, "mmm": multi-model mean, default), needs to be consistent with calc\_IAV\_hatching.ncl
- percent: determines if difference expressed in percent (0, 1, default = 0)
- 6. Script calc\_pattern\_intermodel\_stddev\_scaleT.ncl

- · scenarios: list with scenarios included in figure
- periods: list with start years of periods to be included
- time\_avg: time\_avg: time averaging ("annualclim", "seasonalclim")
- 7. Script calc\_pattern\_interscenario\_stddev\_scaleT.ncl

Required settings for script

- scenarios: list with scenarios included in figure
- periods: list with start years of periods to be included
- time\_avg: time\_avg: time averaging ("annualclim", "seasonalclim")
- 8. Script calc\_pattern\_stddev\_scaleT.ncl

Required settings for script

- scenarios: list with scenarios included in figure
- periods: list with start years of periods to be included
- time\_avg: time\_avg: time averaging ("annualclim", "seasonalclim")
- 9. Script calc\_pattern\_comparison.ncl

Required settings for script

- scenarios: list with two scenarios included in figure. The last scenario is taken as reference. For example to compute the difference of pattern between SSP4-6.0 and SSP4-3.4, the scenario ssp460 should be the last element of the list.
- · periods: list with start years of periods to be included
- time\_avg: time\_avg: time averaging ("annualclim", "seasonalclim")
- label: label of periods
- 10. Script calc\_table\_changes.ncl

Required settings for script

- scenarios: list with scenarios included in the table
- syears: list with start years of time periods to include in the table
- eyears: list with end years of the time periods to include in the table
- begin\_ref\_year: start year of historical baseline period (e.g. 1995)
- end\_ref\_year: end year of historical baseline period (e.g. 2014)
- spread: multiplier of standard deviation to calculate spread with (e.g. 1.64)
- label: list of scenario names included in the table

- 11. Script calc\_table\_warming\_level.ncl
  - Required settings for script
    - scenarios: list with scenarios included in the table
    - warming\_levels: list of warming levels to include in the table
    - syears: list with start years of time periods (historical then SSPs)
    - eyears: list with end years of the time periods (historical then SSPs)
    - begin\_ref\_year: start year of historical baseline period (e.g. 1995)
    - end\_ref\_year: end year of historical baseline period (e.g. 2014)
    - offset: offset between current historical baseline and 1850-1900 period
    - label: list of scenario names included in the table
- 12. Script calc\_timeseries\_mean\_spread\_runave.ncl

- scenarios: list of scenarios to include
- syears: list with start years of time periods (historical then SSPs)
- eyears: list with end years of the time periods (historical then SSPs)
- begin\_ref\_year: start year of historical baseline period (e.g. 1986)
- end\_ref\_year: end year of historical baseline period (e.g. 2005)

#### Optional settings for script

- runave\_window: size of the window used to perform running average (default 11)
- spread: how many standard deviations to calculate the spread with (default 1)
- label: list of scenario names included in the legend
- percent: determines if difference expressed in percent (0, 1, default = 0)
- model\_nr: whether to save number of models used for each scenario
- 13. Script calc\_timeseries\_mean\_spread\_ssp4.ncl

#### Required settings for script

- scenarios: list of scenarios to include: ssp434 and ssp460
- syears: list with start years of time periods (historical then SSPs)
- eyears: list with end years of the time periods (historical then SSPs)
- begin\_ref\_year: start year of historical baseline period (e.g. 1986)
- end\_ref\_year: end year of historical baseline period (e.g. 2005)

- runave\_window: size of the window used to perform running average (default 11)
- spread: how many standard deviations to calculate the spread with (default 1)
- label: list of scenario names included in the legend
- percent: determines if difference expressed in percent (0, 1, default = 0)
- model\_nr: whether to save number of models used for each scenario

- 14. Script calc\_timeseries\_mean\_spread\_ssp5.ncl
  - Required settings for script
    - scenarios: list of scenarios to include: ssp534-over, ssp585
    - syears: list with start years of time periods (historical then SSPs)
    - eyears: list with end years of the time periods (historical then SSPs)
    - begin\_ref\_year: start year of historical baseline period (e.g. 1986)
    - end\_ref\_year: end year of historical baseline period (e.g. 2005)

- runave\_window: size of the window used to perform running average (default 11)
- spread: how many standard deviations to calculate the spread with (default 1)
- · label: list of scenario names included in the legend
- percent: determines if difference expressed in percent (0, 1, default = 0)
- model\_nr: whether to save number of models used for each scenario
- 15. Script plot\_pattern.ncl

Required settings for script

- · scenarios: list of scenarios
- · periods: list with start years of periods
- ancestors: variable and diagnostics that calculated field to be plotted

#### Optional settings for script

- projection: map projection, any valid ncl projection, default = Robinson
- diff\_levs: list with explicit levels for all contour plots
- max\_vert: maximum number of plots in vertical
- max\_hori: maximum number of plots in horizontal
- model\_nr: save number of model runs per period and scenario in netcdf to print in plot? (True, False, default = False)
- colormap: alternative colormap, path to rgb file or ncl name
- span: span whole colormap? (True, False, default = True)
- pltname: alternative name for output plot, default is diagnostic + varname + time\_avg
- units: units written next to colorbar, e.g. (~F35~J~F~C)
- sig: plot stippling for significance? (True, False)
- not\_sig: plot hatching for uncertainty? (True, False)
- label: label to add in the legend
- 16. Script plot\_table\_changes.ncl

Required settings for script

- ancestors: variable and diagnostics that calculated field to be plotted
- · scenarios: list of scenarios included in the figure

- · syears: list of start years of periods of interest
- eyears: list of end years of periods of interest
- label: list of labels of the scenarios

- title: title of the plot
- 17. Script plot\_table\_warming\_level.ncl

#### Required settings for script

- · scenarios: list of scenarios included in the figure
- warming\_levels: list of warming levels
- syears: list of start years of historical and SSPs scenarios
- · eyears: list of end years of historical and SSPs scenarios
- begin\_ref\_year: start year of reference period
- end\_ref\_year: end year of reference period
- label: list of labels of the scenarios
- offset: offset between reference baseline and 1850-1900
- 18. Script plot\_timeseries\_mean\_spread\_3scenarios.ncl

#### Required settings for script

- ancestors: variable and diagnostics that calculated field to be plotted
- scenarios: list of scenarios included in the figure
- · syears: list of start years of historical and SSPs scenarios
- eyears: list of end years of historical and SSPs scenarios
- begin\_ref\_year: start year of reference period
- end\_ref\_year: end year of reference period
- label: list of labels of the scenarios

#### Optional settings for script

- title: specify plot title
- yaxis: specify y-axis title
- ymin: minimim value on y-axis, default calculated from data
- ymax: maximum value on y-axis
- colormap: alternative colormap, path to rgb file or ncl name
- model\_nr: save number of model runs per period and scenario
- styleset: color style
- spread: how many standard deviations to calculate the spread with, default is 1, ipcc tas is 1.64
- 19. Script plot\_timeseries\_mean\_spread\_constrained\_projections.ncl

#### Required settings for script

• ancestors: variable and diagnostics that calculated field to be plotted

- · scenarios: list of scenarios included in the figure
- · syears: list of start years of historical and SSPs scenarios
- · eyears: list of end years of historical and SSPs scenarios
- begin\_ref\_year: start year of reference period
- end\_ref\_year: end year of reference period
- · label: list of labels of the scenarios
- baseline\_offset: offset between reference period (baseline) and 1850-1900
- lower\_constrained\_projections: list of lower bounds of the constrained projections for the scenarios included in the same order as the scenarios
- upper\_constrained\_projections: list of upper bounds of the constrained projections for the scenarios included in the same order as the scenarios
- mean\_constrained\_projections: list of means of the constrained projections for the scenarios included in the same order as the scenarios

- title: specify plot title
- yaxis: specify y-axis title
- ymin: minimim value on y-axis, default calculated from data
- ymax: maximum value on y-axis
- colormap: alternative colormap, path to rgb file or ncl name
- · model\_nr: save number of model runs per period and scenario
- · styleset: color style
- spread: how many standard deviations to calculate the spread with, default is 1, ipcc tas is 1.64
- 20. Script plot\_timeseries\_mean\_spread.ncl

#### Required settings for script

- ancestors: variable and diagnostics that calculated field to be plotted
- · scenarios: list of scenarios included in the figure
- · syears: list of start years of historical and SSPs scenarios
- · eyears: list of end years of historical and SSPs scenarios
- begin\_ref\_year: start year of reference period
- end\_ref\_year: end year of reference period
- label: list of labels of the scenarios

- title: specify plot title
- yaxis: specify y-axis title
- ymin: minimim value on y-axis, default calculated from data
- ymax: maximum value on y-axis
- colormap: alternative colormap, path to rgb file or ncl name

- model\_nr: save number of model runs per period and scenario
- styleset: color style
- spread: how many standard deviations to calculate the spread with, default is 1, ipcc tas is 1.64
- 21. Script plot\_timeseries\_mean\_spread\_rightaxis\_5scen.ncl

- ancestors: variable and diagnostics that calculated field to be plotted
- scenarios: list of scenarios included in the figure
- syears: list of start years of historical and SSPs scenarios
- eyears: list of end years of historical and SSPs scenarios
- begin\_ref\_year: start year of reference period
- end\_ref\_year: end year of reference period
- rightaxis\_offset: offset of the right axis relative to the left axis
- label: list of labels of the scenarios

Optional settings for script

- title: specify plot title
- yaxis: specify y-axis title
- ymin: minimim value on y-axis, default calculated from data
- ymax: maximum value on y-axis
- colormap: alternative colormap, path to rgb file or ncl name
- model\_nr: save number of model runs per period and scenario
- styleset: color style
- spread: how many standard deviations to calculate the spread with, default is 1, ipcc tas is 1.64
- 22. Script plot\_timeseries\_mean\_spread\_ssp4.ncl

Required settings for script

- ancestors: variable and diagnostics that calculated field to be plotted
- · scenarios: list of scenarios included in the figure
- syears: list of start years of historical and SSPs scenarios
- eyears: list of end years of historical and SSPs scenarios
- begin\_ref\_year: start year of reference period
- end\_ref\_year: end year of reference period
- label: list of labels of the scenarios

- title: specify plot title
- yaxis: specify y-axis title
- ymin: minimim value on y-axis, default calculated from data
- ymax: maximum value on y-axis

- colormap: alternative colormap, path to rgb file or ncl name
- model\_nr: save number of model runs per period and scenario
- styleset: color style
- spread: how many standard deviations to calculate the spread with, default is 1, ipcc tas is 1.64
- 23. Script plot\_timeseries\_mean\_spread\_ssp5.ncl

- ancestors: variable and diagnostics that calculated field to be plotted
- · scenarios: list of scenarios included in the figure
- · syears: list of start years of historical and SSPs scenarios
- · eyears: list of end years of historical and SSPs scenarios
- begin\_ref\_year: start year of reference period
- end\_ref\_year: end year of reference period
- · label: list of labels of the scenarios

Optional settings for script

- title: specify plot title
- yaxis: specify y-axis title
- ymin: minimim value on y-axis, default calculated from data
- ymax: maximum value on y-axis
- colormap: alternative colormap, path to rgb file or ncl name
- · model\_nr: save number of model runs per period and scenario
- styleset: color style
- spread: how many standard deviations to calculate the spread with, default is 1, ipcc tas is 1.64
- 24. Script plot\_timeseries\_across\_realization\_stddev\_runave.ncl

Required settings for script

- ancestors: variable and diagnostics that calculated field to be plotted
- · scenarios: list of scenarios included in the figure
- · syears: list of start years of historical and SSPs scenarios
- · eyears: list of end years of historical and SSPs scenarios
- begin\_ref\_year: start year of reference period
- end\_ref\_year: end year of reference period
- label: list of labels of the scenarios
- n\_samples: number of samples of size 10 to draw among all the ensembles of sampled\_model only
- sampled\_model: name of dataset on which to sample

- trend: whether the trend is calculated and displayed
- runave\_window: only used if trend is true, size window used for the centered running average

- title: specify plot title
- yaxis: specify y-axis title
- ymin: minimim value on y-axis, default calculated from data
- ymax: maximum value on y-axis
- colormap: alternative colormap, path to rgb file or ncl name

## 17.15.4 Variables

*Note: These are the variables tested and used in the original paper.* 

- tas (atmos, monthly mean, longitude latitude time)
- pr (atmos, monthly mean, longitude latitude time)

However, the code is flexible and in theory other variables of the same kind can be used.

### 17.15.5 References

Tebaldi, C., Debeire, K., Eyring, V., Fischer, E., Fyfe, J., Friedlingstein, P., Knutti, R., Lowe, J., O'Neill, B., Sanderson, B., van Vuuren, D., Riahi, K., Meinshausen, M., Nicholls, Z., Hurtt, G., Kriegler, E., Lamarque, J.-F., Meehl, G., Moss, R., Bauer, S. E., Boucher, O., Brovkin, V., Golaz, J.-C., Gualdi, S., Guo, H., John, J. G., Kharin, S., Koshiro, T., Ma, L., Olivié, D., Panickal, S., Qiao, F., Rosenbloom, N., Schupfner, M., Seferian, R., Song, Z., Steger, C., Sellar, A., Swart, N., Tachiiri, K., Tatebe, H., Voldoire, A., Volodin, E., Wyser, K., Xin, X., Xinyao, R., Yang, S., Yu, Y., and Ziehn, T.: Climate model projections from the Scenario Model Intercomparison Project (ScenarioMIP) of CMIP6, Earth Syst. Dynam., 12, 253-293, https://doi.org/10.5194/esd-12-253-2021

## 17.15.6 Example plots

# 17.16 Climate Change Hotspot

### 17.16.1 Overview

In the context of a changing climate, it is found that not all regions change at the same pace and the same way. The regions that change at a faster rate than the rest of the globe are labelled as climate change hotspots. Estimating the location and magnitude of the hotspots is important for climate change adaptation, and it is usually computed using the projected climate variables' differences between the regional and larger scales.

One issue when trying to evaluate projections of climate change is the vast amount of information available from the Coupled Model Intercomparison Project (CMIP) exercises. Additionally, results from the CMIP phases 5 and 6 can be quite different, therefore a comparison between the two multi-model ensembles can be made to evaluate their differences and similarities. To account for the projections scenario uncertainty, data from three different end-of-the-century radiative forcings is given in the recipe.

This recipe compares regional surface temperature and precipitation against larger scale means to obtain the hotspot magnitudes for both CMIP5 and CMIP6 in the 2.6, 4.5 and 8.5 \$Wm^-2\$ radiative forcings by the year 2100 against the preindustrial Era (RCP2.6, RCP4.5, RCP8.5 for CMIP5 and SSP1-2.6, SSP2-4.5, SSP5-8.5 for CMIP6). Recipe based on the work by Cos et al. (2022).

Note: This recipe is currently set to evaluate the Mediterranean hotspot (with bounds start\_longitude: -10, end\_longitude: 40, start\_latitude: 30, end\_latitude: 45) but it can be set to any other rectangular region.

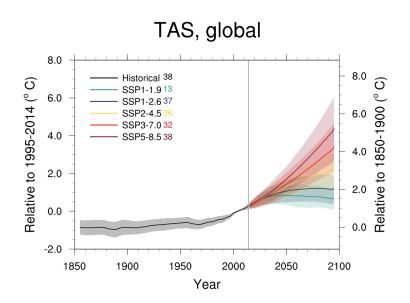
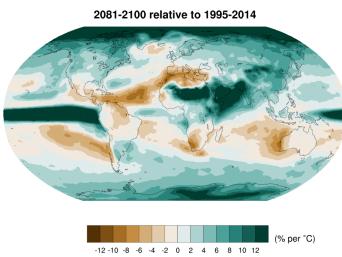


Fig. 48: Global average temperature time series (11-year running averages) of changes from current baseline (1995–2014, left axis) and pre-industrial baseline (1850–1900, right axis, obtained by adding a 0.84 °C offset) for SSP1-1.9, SSP1-2.6, SSP2-4.5, SSP3-7.0 and SSP5-8.5.



Precipitation change scaled by global T

Fig. 49: Patterns of temperature (a) and percent precipitation change (b) normalized by global average temperature change (averaged across CMIP6 models and all Tier 1 plus SSP1-1.9 scenarios).

## 17.16.2 Available recipes and diagnostics

Recipes are stored in esmvaltool/recipes/

• recipe\_climate\_change\_hotspot.yml: Loads and ensembles the data, computes the necessary climate change hotspot diagnostics and plots the results figures.

Diagnostics are stored in esmvaltool/diag\_scripts/cos22esd/

- climate\_change\_hotspot.py: Calculates the regional field hotspot for temperature and precipitation and the 10-year rolling mean timeseries for regional and large-scale temperature and precipitation.
- hotspot\_plotter.py: Gathers the data output from the climate\_change\_hotspot.py script and plots the hotspot fields and the rolling mean timeseries [Figures 2, 3, S2 and S4 by Cos et al. (2022).].

### 17.16.3 User settings in the recipe

Script climate\_change\_hotspot.py

Required settings for script

- baseline\_period: Historical period that serves as a reference to compute the time anomalies.
- future\_periods: List of the two future periods given in years ("YYYY-YYYY") where the hotspot will be computed. Following the format [future period #1, future period #2].
- region: list of longitudes and latitudes that enclose a rectangular region. In the form of [start\_longitude, end\_longitude, start\_latitude, end\_latitude].

	SSP1-1.9	SSP1-2.6	SSP2-4.5	SSP3-7.0	SSP5-8.5
1.5°C warming level	2029	2028	2028	2028	2026
	[2021,NA]	[2020,NA]	[2020,2047]	[2020,2045]	[2020,2040]
	(11/13)	(30/31)	(31/31)	(31/31)	(31/31)
2.0°C warming level	NA	2064	2046	2043	2039
	[2036,NA]	[2032,NA]	[2032,2082]	[2031,2064]	[2030,2055]
	(2/13)	(17/31)	(31/31)	(31/31)	(31/31)
3.0°C warming level	NA	NA	2094	2069	2060
	[NA,NA]	[NA,NA]	[2058,NA]	[2052,NA]	[2048,2083]
	(0/13)	(0/31)	(16/31)	(31/31)	(31/31)
4.0°C warming level	NA	NA	NA	2091	2078
	[NA,NA]	[NA,NA]	[NA,NA]	[2071,NA]	[2062,NA]
	(0/13)	(0/31)	(1/31)	(17/31)	(27/31)
5.0°C warming level	NA	NA	NA	NA	2094
	[NA,NA]	[NA,NA]	[NA,NA]	[2088,NA]	[2075,NA]
	(0/13)	(0/31)	(0/31)	(3/31)	(15/31)

Warming level crossings relative to 1850-1900

Fig. 50: Times (best estimate and range – in square brackets – based on the 5%–95% range of the ensemble after smoothing the trajectories by 11-year running means) at which various warming levels (defined as relative to 1850–1900) are reached according to simulations following, from left to right, SSP1-1.9, SSP1-2.6, SSP2-4.5, SSP3-7.0 and SSP5-8.5. Crossing of these levels is defined by using anomalies with respect to 1995–2014 for the model ensembles and adding the offset of 0.84 to derive warming from pre-industrial values. We use a common subset of 31 models for the Tier 1 scenarios and all available models (13) for SSP1-1.9, while Table A7 shows the result of using all available models under each scenario. The number of models available under each scenario and the number of models reaching a given warming level are shown in parentheses. However, the estimates are based on the ensemble means and ranges computed from all the models considered (13 or 31 in this case), not just from the models that reach a given level. An estimate marked as "NA" is to be interpreted as "not reaching that warming level by 2100". In cases where the ensemble average remains below the warming level for the whole century, it is possible for the central estimate to be NA, while the earlier time of the confidence interval is not, since it is determined by the warmer end of the ensemble range.

- region\_name: Name of the region to be included in the provenance record.
- Script hotspot\_plotter.py

- baseline\_period: Historical period displayed in the figures' titles.
- future\_periods: List of the two future periods given in years ("YYYY-YYYY"), following the format [future period #1, future period #2], used to identify the ancestor files and in the figure titles.
- region: List of longitudes and latitudes that enclose a region. In the form of [start\_longitude, end\_longitude, start\_latitude, end\_latitude]. Used in the title to identify the precipitation large-scale region.
- region\_name: Name of the region used in the plot titles.

#### 17.16.4 Modifying the datasets and scenarios used

recipe\_climate\_change\_hotspot.yml can be modified to use different scenario combinations. The standard recipe uses data from scenarios with the radiative forcings 2.6, 4.5 and 8.5  $Wm^{-2}$  (referred to as 26, 45 and 85), but any combination of three scenarios from the following list can be used:

```
26: "RCP2.6/SSP1-2.6"
45: "RCP4.5/SSP2-4.5"
60: "RCP6.0/SSP4-6.0"
85: "RCP8.5/SSP5-8.5"
```

To specify which datasets are available for each scenario, lists of datasets can be attributed to a specific CMIP project and scenario between the documentation and preprocessor sections of the recipe as follows:

```
cmip6_85: &cmip6_85
   - {...dataset keys...}
   - {...dataset keys...}
cmip5_85: &cmip5_85
   - {...dataset keys...}
   - {...dataset keys...}
cmip6_45: &cmip6_45
   - {...dataset keys...}
cmip5_45: &cmip5_45
   - {...dataset keys...}
   - {...dataset keys...}
   - {...dataset keys...}
```

These different dataset sections will be called at each diagnostic as additional\_datasets using the anchors \*cmip6\_85, \*cmip5\_85, etc. as in the example:

```
pr_cmip6_85:
variables:
    pr:
    mip: Amon
    short_name: pr
    preprocessor: ensemble_members
    additional_datasets: *cmip6_85
scripts:
```

(continues on next page)

(continued from previous page)

```
pr_cmip6_85:
    <<: *script_input</pre>
```

In case of wanting to use other scenarios, the datasets and diagnostics must be changed maintaining the format cmip{phase}\_{scenario} and {variable}\_cmip{phase}\_{scenario}. For example, if we want scenario 60 instead of scenario 85, we would need to include the files available for cmip6\_60 and cmip5\_60, and the previous diagnostic would change to:

```
pr_cmip6_60:
variables:
    pr:
        mip: Amon
        short_name: pr
        preprocessor: ensemble_members
        additional_datasets: *cmip6_60
scripts:
    pr_cmip6_60:
        <<: *script_input</pre>
```

Finally, if the datasets that need to be included in the multi-model means are common for all scenarios, the datasets could be simplified to:

```
cmip6: &cmip6
   - {...dataset keys...}
   - {...dataset keys...}
cmip5: &cmip5
   - {...dataset keys...}
   - {...dataset keys...}
```

Note that the diagnostics' additional\_datasets will need to be modified accordingly.

### 17.16.5 Variables

- tas (atmos, monthly mean, longitude latitude time)
- pr (atmos, monthly mean, longitude latitude time)

#### 17.16.6 References

• Cos et al. 2022, Earth Syst. Dynam., 13, 321-340

### 17.16.7 Example plots

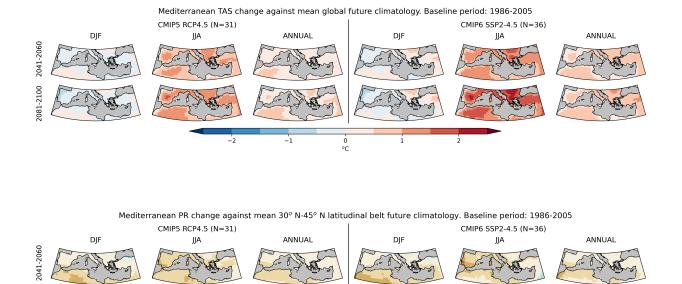


Fig. 51: Mediterranean region temperature (upper rows) and precipitation (lower rows) change differences against the mean global temperature change and the mean 30–45° N latitudinal belt precipitation change respectively. The changes for the periods 2041–2060 (first and third row) and 2081–2100 (second and fourth row) are evaluated against 1986–2005 mean. The differences are shown for the CMIP5 (left) and CMIP6 (right) DJF, JJA and annual mean projections (columns) under the high emission scenario RCP8.5 and SSP5-8.5 respectively. N indicates the number of models included in the ensemble mean.

ò

20

40

-40

-20

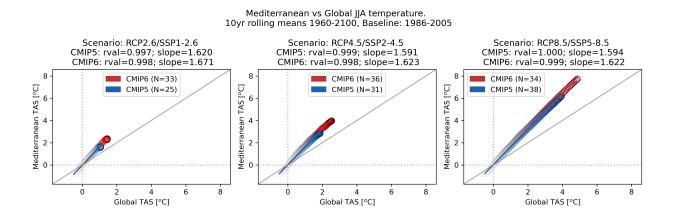


Fig. 52: Mediterranean region warming against global warming for the summer 2.6, 4.5 and 8.5  $Wm^{-2}$  RCP and SSP scenarios for the CMIP5 and CMIP6 ensemble means. Each dot represents a 10-year mean change beginning from the period 1960-1969 (light colouring) until 2091-2100 (opaque coloring). The changes are computed with 1986-2005 as the baseline. An ordinary least squares linear regression is computed and the slope and \$r\$ values are shown. N indicates the number of models included in the ensemble mean.

081-2100

# EIGHTEEN

# IPCC

# 18.1 IPCC AR6 Chapter 3 (selected figures)

#### 18.1.1 Overview

This recipe collects selected diagnostics used in IPCC AR6 WGI Chapter 3: Human influence on the climate system (Eyring et al., 2021). Plots from IPCC AR6 can be readily reproduced and compared to previous versions. The aim is to be able to start with what was available now the next time allowing us to focus on developing more innovative analysis methods rather than constantly having to "re-invent the wheel".

Processing of CMIP3 models currently works only in serial mode, due to an issue in the input data still under investigation. To run the recipe for Fig 3.42a and Fig. 3.43 set "max\_parallel\_tasks: 1" in the config-user.yml file.

The plots are produced collecting the diagnostics from individual recipes. The following figures from Eyring et al. (2021) can currently be reproduced:

- Figure 3.3 a,b,c,d: Surface Air Temperature Model Bias
- Figure 3.4: Anomaly Of Near-Surface Air Temperature
- Figure 3.5: Temporal Variability Of Near-Surface Air Temperature
- Figure 3.9: Anomaly Of Near-Surface Air Temperature Attribution
- Figure 3.13: Precipitation Model Bias
- Figure 3.15: Precipitation Anomaly
- Figure 3.19: Speed-Up Of Zonal Mean Wind
- Figure 3.42: Relative Model Performance
- Figure 3.43: Correlation Pattern

To reproduce Fig. 3.9 you need the shapefile of the AR6 reference regions (Iturbide et al., 2020). Please download the file IPCC-WGI-reference-regions-v4\_shapefile.zip, unzip and store it in *<auxiliary\_data\_dir>/IPCC-regions/* (the *auxiliary\_data\_dir is* defined in the config-user.yml file).

### 18.1.2 Available recipes and diagnostics

Recipes are stored in esmvaltool/recipes/ipccwg1ar6ch3/

- recipe\_ipccwg1ar6ch3\_atmosphere.yml
- recipe\_ipccwg1ar6ch3\_fig\_3\_9.yml
- recipe\_ipccwg1ar6ch3\_fig\_3\_19.yml
- recipe\_ipccwg1ar6ch3\_fig\_3\_42\_a.yml
- recipe\_ipccwg1ar6ch3\_fig\_3\_42\_b.yml
- recipe\_ipccwg1ar6ch3\_fig\_3\_43.yml

Diagnostics are stored in esmvaltool/diag\_scripts/

Fig. 3.3:

- ipcc\_ar5/ch12\_calc\_IAV\_for\_stippandhatch.ncl: See *here*:.
- ipcc\_ar6/model\_bias.ncl

Fig. 3.4:

- ipcc\_ar6/tas\_anom.ncl
- ipcc\_ar6/tsline\_collect.ncl

Fig. 3.5:

ipcc\_ar6/zonal\_st\_dev.ncl

Fig. 3.9:

• ipcc\_ar6/tas\_anom\_damip.ncl

Fig. 3.13:

- ipcc\_ar5/ch12\_calc\_IAV\_for\_stippandhatch.ncl: See *here:*.
- ipcc\_ar6/model\_bias.ncl

Fig. 3.15:

• ipcc\_ar6/precip\_anom.ncl

Fig. 3.19:

• ipcc\_ar6/zonal\_westerly\_winds.ncl

Fig. 3.42:

- perfmetrics/main.ncl
- perfmetrics/collect.ncl

Fig. 3.43:

- ipcc\_ar6/corr\_pattern.ncl
- ipcc\_ar6/corr\_pattern\_collect.ncl

### 18.1.3 User settings in recipe

1. Script ipcc\_ar5/ch12\_calc\_IAV\_for\_stippandhatch.ncl

See here.

2. Script ipcc\_ar6/model\_bias.ncl

Optional settings (scripts)

- plot\_abs\_diff: additionally also plot absolute differences (true, false)
- plot\_rel\_diff: additionally also plot relative differences (true, false)
- plot\_rms\_diff: additionally also plot root mean square differences (true, false)
- projection: map projection, e.g., Mollweide, Mercator
- timemean: time averaging, i.e. "seasonalclim" (DJF, MAM, JJA, SON), "annualclim" (annual mean)

#### Required settings (variables)

• reference\_dataset: name of reference dataset

#### Color tables

- variable "tas" and "tos": diag\_scripts/shared/plot/rgb/ipcc-ar6\_temperature\_div.rgb, diag\_scripts/shared/plot/rgb/ipcc-ar6\_temperature\_10.rgb, diag\_scripts/shared/plot/rgb/ipcc-ar6\_temperature\_seq.rgb
- variable "pr": diag\_scripts/shared/plots/rgb/ipcc-ar6\_precipitation\_seq.rgb, diag\_scripts/shared/plot/rgb/ipcc-ar6\_precipitation\_10.rgb
- variable "sos": diag\_scripts/shared/plot/rgb/ipcc-ar6\_misc\_seq\_1.rgb, diag\_scripts/shared/plot/rgb/ipcc-ar6\_misc\_div.rgb
- 3. Script ipcc\_ar6/tas\_anom.ncl

Required settings for script

• styleset: as in diag\_scripts/shared/plot/style.ncl functions

Optional settings for script

- blending: if true, calculates blended surface temperature
- ref\_start: start year of reference period for anomalies
- ref\_end: end year of reference period for anomalies
- ref\_value: if true, right panel with mean values is attached
- ref\_mask: if true, model fields will be masked by reference fields
- region: name of domain
- plot\_units: variable unit for plotting
- y-min: set min of y-axis
- y-max: set max of y-axis
- header: if true, region name as header
- volcanoes: if true, adds volcanoes to the plot
- write\_stat: if true, write multi model statistics in nc-file

Optional settings for variables

• reference\_dataset: reference dataset; REQUIRED when calculating anomalies

#### Color tables

- e.g. diag\_scripts/shared/plot/styles/cmip5.style
- 4. Script ipcc\_ar6/tas\_anom\_damip.ncl

Required settings for script

- start\_year: start year in figure
- end\_year: end year in figure
- panels: list of variable blocks for each panel

#### Optional settings for script

- ref\_start: start year of reference period for anomalies
- ref\_end: end year of reference period for anomalies
- ref\_mask: if true, model fields will be masked by reference fields
- plot\_units: variable unit for plotting
- y-min: set min of y-axis
- y-max: set max of y-axis
- header: title for each panel
- title: name of region as part of filename
- legend: set labels for optional output of a legend in an extra file
- 5. Script ipcc\_ar6/tsline\_collect.ncl

#### Optional settings for script

- blending: if true, then var="gmst" otherwise "gsat"
- ref\_start: start year of reference period for anomalies
- ref\_end: end year of reference period for anomalies
- region: name of domain
- plot\_units: variable unit for plotting
- y-min: set min of y-axis
- y-max: set max of y-axis
- order: order in which experiments should be plotted
- stat\_shading: if true: shading of statistic range
- ref\_shading: if true: shading of reference period

Optional settings for variables

- reference\_dataset: reference dataset; REQUIRED when calculating anomalies
- 6. Script ipcc\_ar6/zonal\_st\_dev.ncl

Required settings for script

• styleset: as in diag\_scripts/shared/plot/style.ncl functions

- plot\_legend: if true, plot legend will be plotted
- plot\_units: variable unit for plotting
- multi\_model\_mean: if true, multi-model mean and uncertaintiy will be plotted

Optional settings for variables

- reference\_dataset: reference dataset; REQUIRED when calculating anomalies
- 7. Script ipcc\_ar6/precip\_anom.ncl

Required settings for script

- panels: list of variables plotted in each panel
- start\_year: start of time coordinate
- end\_year: end of time coordinate

Optional settings for script

- anomaly: true if anomaly should be calculated
- ref\_start: start year of reference period for anomalies
- ref\_end: end year of reference period for anomalies
- ref\_mask: if true, model fields will be masked by reference fields
- region: name of domain
- plot\_units: variable unit for plotting
- header: if true, region name as header
- stat: statistics for multi model nc-file (MinMax,5-95,10-90)
- y\_min: set min of y-axis
- y\_max: set max of y-axis
- 8. Script ipcc\_ar6/zonal\_westerly\_winds.ncl
  - Optional settings for variables
    - reference\_dataset: reference dataset; REQUIRED when calculating anomalies

Optional settings for script

- e13fig12\_start\_year: year when the climatology calculation starts (default: start\_year of var)
- e13fig12\_end\_year: year when the climatology calculation ends (default: end\_year of var)
- e13fig12\_multimean: multimodel mean (default: False)
- e13fig12\_exp\_MMM: name of the experiments for the MMM (required if @e13fig12\_multimean = True)
- e13fig12\_season: season (default: ANN)
- 9. Script perfmetrics/perfmetrics\_main.ncl

See here.

10. Script perfmetrics/perfmetrics\_collect.ncl

See *here*.

11. Script ipcc\_ar6/corr\_pattern.ncl Required settings for variables

- reference\_dataset: name of reference observation
- Optional settings for variables
  - alternative\_dataset: name of alternative observations
- 12. Script ipcc\_ar6/corr\_pattern\_collect.ncl

- diag\_order: give order of plotting variables on the x-axis
- labels: List of labels for each variable on the x-axis
- model\_spread: if True, model spread is shaded
- plot\_median: if True, median is plotted
- · project\_order: give order of projects

#### 18.1.4 Variables

- et (land, monthly mean, longitude latitude time)
- fgco2 (ocean, monthly mean, longitude latitude time)
- gpp (land, monthly mean, longitude latitude time)
- hfds (land, monthly mean, longitude latitude time)
- hus (land, monthly mean, longitude latitude level time)
- lai (land, monthly mean, longitude latitude time)
- lwcre (atmos, monthly mean, longitude latitude time)
- nbp (land, monthly mean, longitude latitude time)
- pr (atmos, monthly mean, longitude latitude time)
- psl (atmos, monthly mean, longitude latitude time)
- rlds (atmos, monthly mean, longitude latitude time)
- rlus (atmos, monthly mean, longitude latitude time)
- rlut (atmos, monthly mean, longitude latitude time)
- rsds (atmos, monthly mean, longitude latitude time)
- rsus (atmos, monthly mean, longitude latitude time)
- rsut (atmos, monthly mean, longitude latitude time)
- sm (land, monthly mean, longitude latitude time)
- sic (seaice, monthly mean, longitude latitude time)
- siconc (seaice, monthly mean, longitude latitude time)
- swcre (atmos, monthly mean, longitude latitude time)
- ta (atmos, monthly mean, longitude latitude level time)
- tas (atmos, monthly mean, longitude latitude time)
- tasa (atmos, monthly mean, longitude latitude time)
- tos (atmos, monthly mean, longitude latitude time)

- ts (atmos, monthly mean, longitude latitude time)
- ua (atmos, monthly mean, longitude latitude level time)
- va (atmos, monthly mean, longitude latitude level time)
- zg (atmos, monthly mean, longitude latitude level time)

### 18.1.5 Observations and reformat scripts

- AIRS (hus obs4MIPs)
- ATSR (tos obs4MIPs)
- BerkeleyEarth (tasa esmvaltool/cmorizers/data/formatters/datasets/berkeleyearth.py)
- CERES-EBAF (rlds, rlus, rlut, rlutcs, rsds, rsus, rsut, rsutcs obs4MIPs)
- CRU (pr esmvaltool/cmorizers/data/formatters/datasets/cru.py)
- ESACCI-SOILMOISTURE (sm esmvaltool/cmorizers/data/formatters/datasets /esacci\_soilmoisture.py)
- ESACCI-SST (ts esmvaltool/cmorizers/data/formatters/datasets/esacci\_sst.py)
- ERA5 (hus, psl, ta, tas, ua, va, zg ERA5 data can be used via the native6 project)
- ERA-Interim (hfds cmorizers/data/formatters/datasets/era\_interim.py)
- FLUXCOM (gpp cmorizers/data/formatters/datasets/fluxcom.py)
- GHCN (pr esmvaltool/cmorizers/data/formatters/datasets/ghcn.ncl)
- GPCP-SG (pr obs4MIPs)
- HadCRUT5 (tasa esmvaltool/cmorizers/data/formatters/datasets/hadcrut5.py)
- HadISST (sic, tos, ts esmvaltool/cmorizers/data/formatters/datasets/hadisst.ncl)
- JMA-TRANSCOM (fgco2, nbp esmvaltool/cmorizers/data/formatters/datasets/jma\_transcom.py)
- JRA-55 (psl ana4MIPs)
- Kadow2020 (tasa esmvaltool/cmorizers/data/formatters/datasets/kadow2020.py)
- LandFlux-EVAL (et esmvaltool/cmorizers/data/formatters/datasets/landflux\_eval.py)
- Landschuetzer2016 (fgco2 esmvaltool/cmorizers/data/formatters/datasets/landschuetzer2016.py)
- LAI3g (lai esmvaltool/cmorizers/data/formatters/datasets/lai3g.py)
- MTE (gpp esmvaltool/cmorizers/data/formatters/datasets/mte.py)
- NCEP-NCAR-R1 (ta, tas, ua, va, zg esmvaltool/cmorizers/data/formatters/datasets/ncep\_ncar\_r1.py)
- NOAAGlobalTemp (tasa esmvaltool/cmorizers/data/formatters/datasets/noaaglobaltemp.py)

### 18.1.6 References

Eyring, V., N.P. Gillett, K.M. Achuta Rao, R. Barimalala, M. Barreiro Parrillo, N. Bellouin, C. Cassou, P.J. Durack, Y. Kosaka, S. McGregor, S. Min, O. Morgenstern, and Y. Sun, 2021: Human Influence on the Climate System. In Climate Change 2021: The Physical Science Basis. Contribution of Working Group I to the Sixth Assessment Report of the Intergovernmental Panel on Climate Change [Masson-Delmotte, V., P. Zhai, A. Pirani, S.L. Connors, C. Péan, S. Berger, N. Caud, Y. Chen, L. Goldfarb, M.I. Gomis, M. Huang, K. Leitzell, E. Lonnoy, J.B.R. Matthews, T.K. Maycock, T. Waterfield, O. Yelekçi, R. Yu, and B. Zhou (eds.)]. Cambridge University Press, Cambridge, United Kingdom and New York, NY, USA, pp. 423-552, doi: 10.1017/9781009157896.005.

## 18.1.7 Example plots

# 18.2 IPCC AR5 Chapter 9 (selected figures)

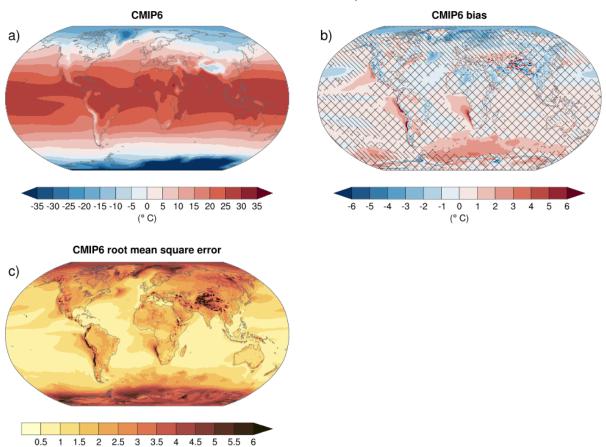
### 18.2.1 Overview

The goal of this recipe is to collect diagnostics to reproduce Chapter 9 of AR5, so that the plots can be readily reproduced and compared to previous CMIP versions. In this way we can next time start with what was available in the previous round and can focus on developing more innovative methods of analysis rather than constantly having to "re-invent the wheel".

**Note:** Please note that most recipes have been modified to include only models that are (still) readily available via ESGF. Plots produced may therefore look different than the original figures from IPCC AR5.

The plots are produced collecting the diagnostics from individual recipes. The following figures from Flato et al. (2013) can currently be reproduced:

- Figure 9.2 a,b,c: Annual-mean surface air temperature for the period 1980-2005. a) multi-model mean, b) bias as the difference between the CMIP5 multi-model mean and the climatology from ERA-Interim (Dee et al., 2011), c) mean absolute model error with respect to the climatology from ERA-Interim.
- Figure 9.3: Seasonality (December-January-February minus June-July-August) of surface (2 m) air temperature (°C) for the period 1980-2005. (a) Multi-model mean for the historical experiment. (b) Multi-model mean of absolute seasonality. (c) Difference between the multi-model mean and the ERA-Interim reanalysis seasonality. (d) Difference between the multi-model mean and the ERA-Interim absolute seasonality.
- Figure 9.4: Annual-mean precipitation rate (mm day-1) for the period 1980-2005. a) multi-model mean, b) bias as the difference between the CMIP5 multi-model mean and the climatology from the Global Precipitation Climatology Project (Adler et al., 2003), c) multi-model mean absolute error with respect to observations, and d) multi-model mean error relative to the multi-model mean precipitation itself.
- Figure 9.5: Climatological (1985-2005) annual-mean cloud radiative effects in Wm-2 for the CMIP5 models against CERES EBAF (2001-2011) in Wm-2. Top row shows the shortwave effect; middle row the longwave effect, and bottom row the net effect. Multi-model-mean biases against CERES EBAF 2.6 are shown on the left, whereas the right panels show zonal averages from CERES EBAF 2.6 (black), the individual CMIP5 models (thin gray lines), and the multi-model mean (thick red line).
- Figure 9.6: Centered pattern correlations between models and observations for the annual mean climatology over the period 1980–1999. Results are shown for individual CMIP3 (black) and CMIP5 (blue) models as thin dashes, along with the corresponding ensemble average (thick dash) and median (open circle). The four variables shown are surface air temperature (TAS), top of the atmosphere (TOA) outgoing longwave radiation (RLUT), precipitation (PR) and TOA shortwave cloud radiative effect (SW CRE). The correlations between the reference and alternate observations are also shown (solid green circles).



## Near-Surface Air Temperature

Fig. 1: Figure 3.3: Annual mean near-surface (2 m) air temperature (°C) for the period 1995-2014. (a) Multi-model (ensemble) mean constructed with one realization of the CMIP6 historical experiment from each model. (b) Multi-model mean bias, defined as the difference between the CMIP6 multi-model mean and the climatology of the fifth generation European Centre for Medium-Range Weather Forecasts (ECMWF) atmospheric reanalysis of the global climate (ERA5). (c) Multi-model mean of the root mean square error calculated over all months separately and averaged, with respect to the climatology from ERA5. Uncertainty is represented using the advanced approach: No overlay indicates regions with robust signal, where >=66% of models show change greater than the variability threshold and >=80% of all models agree on sign of change; diagonal lines indicate regions with no change or no robust signal, where <66% of models show a change greater than the variability threshold; crossed lines indicate regions with conflicting signal, where >=66% of models show change greater than the variability threshold and <80% of all models agree on sign of change.

(° C)

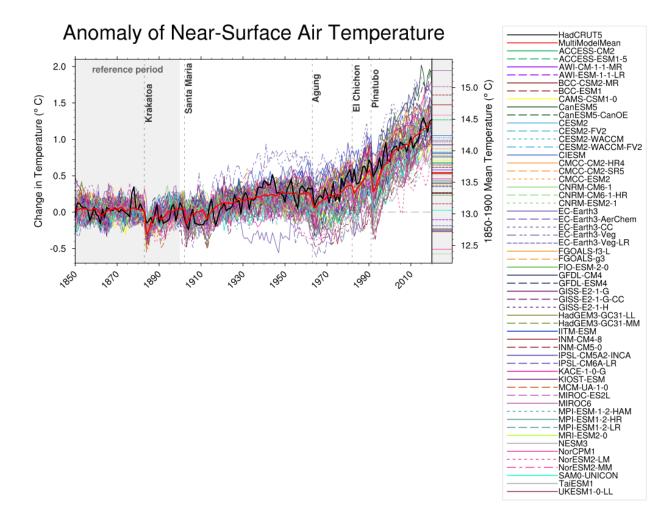


Fig. 2: Figure 3.4a: Observed and simulated time series of the anomalies in annual and global mean surface air temperature (GSAT). All anomalies are differences from the 1850-1900 time-mean of each individual time series. The reference period 1850-1900 is indicated by grey shading. (a) Single simulations from CMIP6 models (thin lines) and the multi-model mean (thick red line). Observational data (thick black lines) are from the Met Office Hadley Centre/Climatic Research Unit dataset (HadCRUT5), and are blended surface temperature (2 m air temperature over land and sea surface temperature over the ocean). All models have been subsampled using the HadCRUT5 observational data mask. Vertical lines indicate large historical volcanic eruptions. Inset: GSAT for each model over the reference period, not masked to any observations.

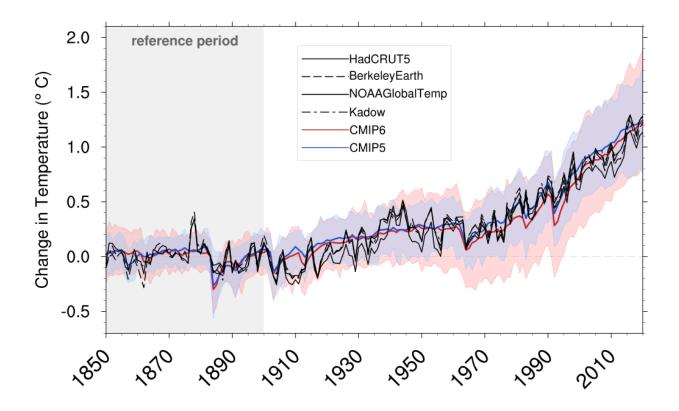
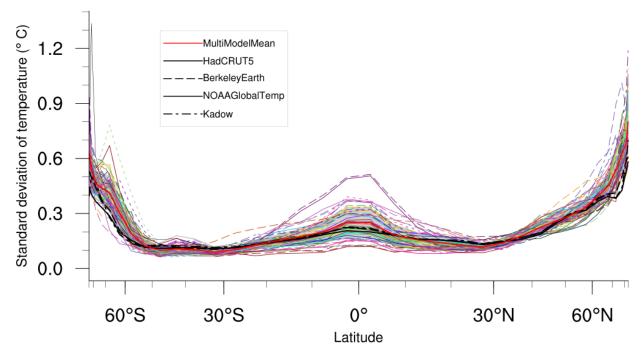


Fig. 3: Figure 3.4b: Observed and simulated time series of the anomalies in annual and global mean surface air temperature (GSAT). All anomalies are differences from the 1850-1900 time-mean of each individual time series. The reference period 1850-1900 is indicated by grey shading. (b) Multi-model means of CMIP5 (blue line) and CMIP6 (red line) ensembles and associated 5th to 95th percentile ranges (shaded regions). Observational data are HadCRUT5, Berkeley Earth, National Oceanic and Atmospheric Administration NOAAGlobalTemp and Kadow et al. (2020). Masking was done as in (a). CMIP6 historical simulations were extended with SSP2-4.5 simulations for the period 2015-2020 and CMIP5 simulations were extended with RCP4.5 simulations for the period 2006-2020. All available ensemble members were used. The multi-model means and percentiles were calculated solely from simulations available for the whole time span (1850-2020).



# Temporal variability of near-surface air temperature

Fig. 4: Figure 3.5: The standard deviation of annually averaged zonal-mean near-surface air temperature. This is shown for four detrended observed temperature datasets (HadCRUT5, Berkeley Earth, NOAAGlobalTemp and Kadow et al. (2020), for the years 1995-2014) and 59 CMIP6 pre-industrial control simulations (one ensemble member per model, 65 years) (after Jones et al., 2013). For line colours see the legend of Figure 3.4. Additionally, the multi-model mean (red) and standard deviation (grey shading) are shown. Observational and model datasets were detrended by removing the least-squares quadratic trend.

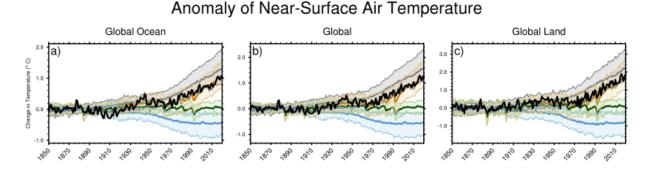
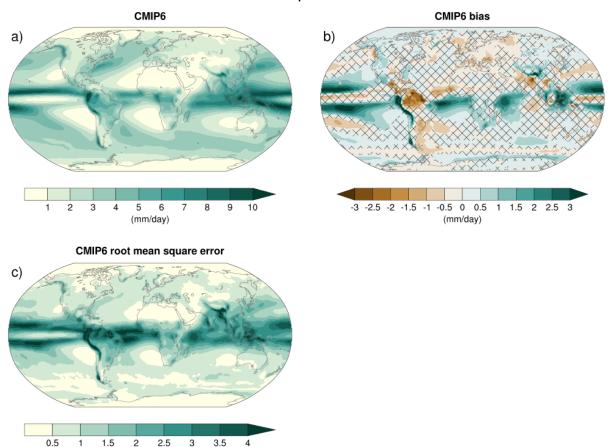


Fig. 5: Figure 3.9: Global, land and ocean annual mean near-surface air temperature anomalies in CMIP6 models and observations. Timeseries are shown for CMIP6 historical anthropogenic and natural (brown) natural-only (green), greenhouse gas only (grey) and aerosol only (blue) simulations (multi-model means shown as thick lines, and shaded ranges between the 5th and 95th percentiles) and for HadCRUT5 (black). All models have been subsampled using the HadCRUT5 observational data mask. Temperature anomalies are shown relative to 1950-2010 for Antarctica and relative to 1850-1900 for other continents. CMIP6 historical simulations are expanded by the SSP2-4.5 scenario simulations. All available ensemble members were used. Regions are defined by Iturbide et al. (2020).

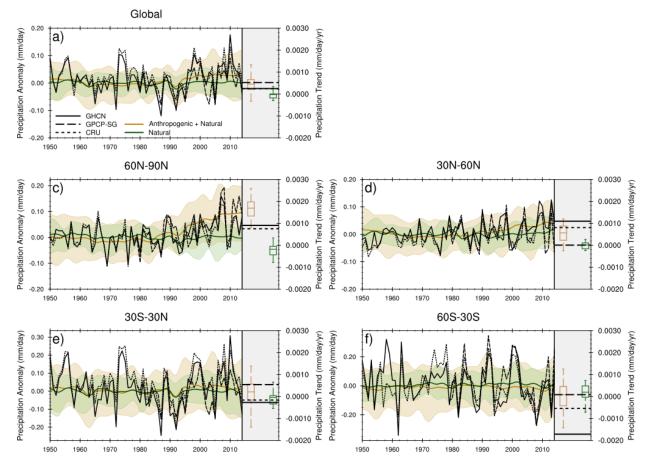
- Figure 9.8: Observed and simulated time series of the anomalies in annual and global mean surface temperature. All anomalies are differences from the 1961-1990 time-mean of each individual time series. The reference period 1961-1990 is indicated by yellow shading; vertical dashed grey lines represent times of major volcanic eruptions. Single simulations for CMIP5 models (thin lines); multi-model mean (thick red line); different observations (thick black lines). Dataset pre-processing like described in Jones et al., 2013.
- Figure 9.14: Sea surface temperature plots for zonal mean error, equatorial (5 deg north to 5 deg south) mean error, and multi model mean for zonal error and equatorial mean.
- Figure 9.24: Time series of (a) Arctic and (b) Antarctic sea ice extent; trend distributions of (c) September Arctic and (d) February Antarctic sea ice extent.
- Figure 9.26: Ensemble-mean global ocean carbon uptake (a) and global land carbon uptake (b) in the CMIP5 ESMs for the historical period 1900–2005. For comparison, the observation-based estimates provided by the Global Carbon Project (GCP) are also shown (thick black line). The confidence limits on the ensemble mean are derived by assuming that the CMIP5 models are drawn from a t-distribution. The grey areas show the range of annual mean fluxes simulated across the model ensemble. This figure includes results from all CMIP5 models that reported land CO2 fluxes, ocean CO2 fluxes, or both (Anav et al., 2013).
- Figure 9.27: Simulation of global mean (a) atmosphere–ocean CO2 fluxes ("fgCO2") and (b) net atmosphere–land CO2 fluxes ("NBP"), by ESMs for the period 1986–2005. For comparison, the observation-based estimates provided by Global Carbon Project (GCP) and the Japanese Meteorological Agency (JMA) atmospheric inversion are also shown. The error bars for the ESMs and observations represent interannual variability in the fluxes, calculated as the standard deviation of the annual means over the period 1986–2005.
- Figure 9.38: Seasonal cycle for the surface temperature or precipitation over land within defined regions multimodel mean and difference to reference dataset or absolute annual cycle can be chosen.
- Figure 9.39: Seasonal bias box and whiskers plot for surface temperature or precipitation within SREX (IPCC Special Report on Managing the Risks of Extreme Events and Disasters to Advance Climate Change Adaptation) regions.
- Figure 9.40: Seasonal bias box and whiskers plot for surface temperature or precipitation within defined polar and ocean regions.
- Figure 9.41b: Comparison between observations and models for variable values within defined regions.



Precipitation

Fig. 6: Figure 3.13: Annual-mean precipitation rate (mm day-1) for the period 1995-2014. (a) Multi-model (ensemble) mean constructed with one realization of the CMIP6 historical experiment from each model. (b) Multi-model mean bias, defined as the difference between the CMIP6 multi-model mean and precipitation analysis from the Global Precipitation Climatology Project (GPCP) version 2.3 (Adler et al., 2003). (c) Multi-model mean of the root mean square error calculated over all months separately and averaged with respect to the precipitation analysis from GPCP version 2.3. Uncertainty is represented using the advanced approach. No overlay indicates regions with robust signal, where  $\geq 66\%$  of models show change greater than the variability threshold and  $\geq 80\%$  of all models agree on sign of change; diagonal lines indicate regions with no change or no robust signal, where < 66% of models show a change greater than the variability threshold and  $\geq 80\%$  of models show a change greater than the variability threshold and < 80% of all models agree on sign of change greater than the variability threshold agree on the sign of change.

(mm/day)



# **Precipitation Anomaly**

Fig. 7: Figure 3.15: Observed and simulated time series of anomalies in zonal average annual mean precipitation. (a), (c-f) Evolution of global and zonal average annual mean precipitation (mm day-1) over areas of land where there are observations, expressed relative to the base period of 1961-1990, simulated by CMIP6 models (one ensemble member per model) forced with both anthropogenic and natural forcings (brown) and natural forcings only (green). Multi-model means are shown in thick solid lines and shading shows the 5-95% confidence interval of the individual model simulations. The data is smoothed using a low pass filter. Observations from three different datasets are included: gridded values derived from Global Historical Climatology Network (GHCN version 2) station data, updated from Zhang et al. (2007), data from the Global Precipitation Climatology Product (GPCP L3 version 2.3, Adler et al. (2003)) and from the Climate Research Unit (CRU TS4.02, Harris et al. (2014)). Also plotted are boxplots showing interquartile and 5-95% ranges of simulated trends over the period for simulations forced with both anthropogenic and natural forcings (brown) and natural forcings only (blue). Observed trends for each observational product are shown as horizontal lines. Panel (b) shows annual mean precipitation rate (mm day-1) of GHCN version 2 for the years 1950-2014 over land areas used to compute the plots.

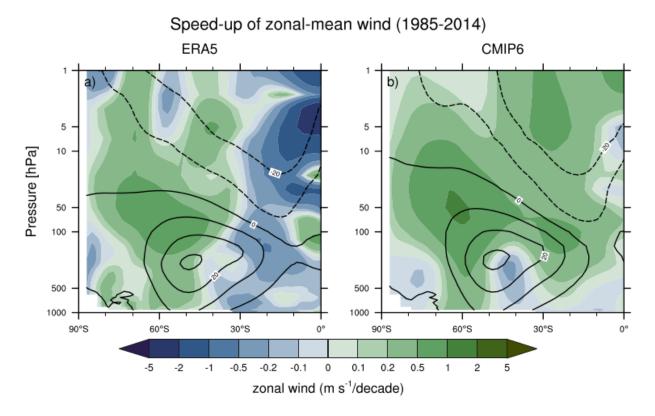


Fig. 8: Figure 3.19: Long-term mean (thin black contours) and linear trend (colour) of zonal mean December-January-February zonal winds from 1985 to 2014 in the Southern Hemisphere. The figure shows (a) ERA5 and (b) the CMIP6 multi-model mean (58 CMIP6 models). The solid contours show positive (westerly) and zero long-term mean zonal wind, and the dashed contours show negative (easterly) long-term mean zonal wind. Only one ensemble member per model is included. Figure is modified from Eyring et al. (2013), their Figure 12.

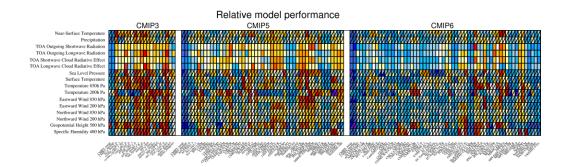


Fig. 9: Figure 3.42a: Relative space-time root-mean-square deviation (RMSD) calculated from the climatological seasonal cycle of the CMIP simulations (1980-1999) compared to observational datasets. A relative performance measure is displayed, with blue shading indicating better and red shading indicating worse performance than the median error of all model results. A diagonal split of a grid square shows the relative error with respect to the reference data set (lower right triangle) and an additional data set (upper left triangle). Reference/additional datasets are from top to bottom in (a): ERA5/NCEP, GPCP-SG/GHCN, CERES-EBAF, CERES-EBAF, CERES-EBAF, CERES-EBAF, JRA-55/ERA5, ESACCI-SST/HadISST, ERA5/NCEP, ERA5/

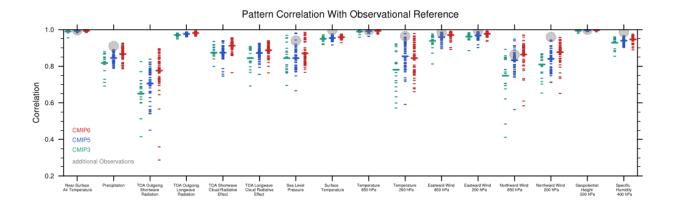


Fig. 10: Figure 3.43 | Centred pattern correlations between models and observations for the annual mean climatology over the period 1980-1999. Results are shown for individual CMIP3 (green), CMIP5 (blue) and CMIP6 (red) models (one ensemble member from each model is used) as short lines, along with the corresponding multi-model ensemble averages (long lines). Correlations are shown between the models and the primary reference observational data set (from left to right: ERA5, GPCP-SG, CERES-EBAF, CERES-EBAF, CERES-EBAF, CERES-EBAF, JRA-55, ESACCI-SST, ERA5, AIRS, ERA5). In addition, the correlation between the primary reference and additional observational datasets (from left to right: NCEP, GHCN, -, -, -, ERA5, HadISST, NCEP, Searce and additions, the pattern correlations are computed after regridding all datasets to a resolution of 4° in longitude and 5° latitude.

- Figure 9.42a: Equilibrium climate sensitivity (ECS) against the global mean surface air temperature, both for the period 1961-1990 and for the pre-industrial control runs.
- Figure 9.42b: Transient climate response (TCR) against equilibrium climate sensitivity (ECS).
- Figure 9.45a: Scatterplot of springtime snow-albedo effect values in climate change vs. springtime  $d(alpha_s)/d(T_s)$  values in the seasonal cycle in transient climate change experiments (Hall and Qu, 2006).

# 18.2.2 Available recipes and diagnostics

Recipes are stored in esmvaltool/recipes/recipe\_ipccwg1ar5ch9

- recipe\_flato13ipcc\_figures\_92\_95.yml: Figures 9.2, 9.3, 9.4, 9.5
- recipe\_flato13ipcc\_figure\_96.yml: Figure 9.6
- recipe\_flato13ipcc\_figure\_98.yml: Figure 9.8
- recipe\_flato13ipcc\_figure\_914.yml: Figure 9.14
- recipe\_flato13ipcc\_figure\_924.yml: Figure 9.24
- recipe\_flato13ipcc\_figures\_926\_927.yml: Figures 9.26 and 9.27
- recipe\_flato13ipcc\_figure\_942.yml: Figure 9.42
- recipe\_flato13ipcc\_figure\_945a.yml: Figure 9.45a
- recipe\_flato13ipcc\_figures\_938\_941\_cmip3.yml: Figures 9.38, 9.39, 9.40, and 9.41
- recipe\_flato13ipcc\_figures\_938\_941\_cmip6.yml: Figures 9.38, 9.39, 9.40, and 9.41 CMIP6 instead of CMIP3

• recipe\_weigel21gmd\_figures\_13\_16.yml: ESMValTool paper version (Weigel et al., 2021) of Figures 9.38, 9.39, 9.40, and 9.41, only CMIP5

Diagnostics are stored in esmvaltool/diag\_scripts/

- carbon\_cycle/main.ncl: See here.
- climate\_metrics/ecs.py: See here.
- clouds/clouds\_bias.ncl: global maps of the multi-model mean and the multi-model mean bias (Fig. 9.2, 9.4)
- clouds/clouds\_ipcc.ncl: global maps of multi-model mean minus observations + zonal averages of individual models, multi-model mean and observations (Fig. 9.5)
- ipcc\_ar5/ch09\_fig09\_3.ncl: multi-model mean seasonality of near-surface temperature (Fig. 9.3)
- ipcc\_ar5/ch09\_fig09\_6.ncl: calculating pattern correlations of annual mean climatologies for one variable (Fig 9.6 preprocessing)
- ipcc\_ar5/ch09\_fig09\_6\_collect.ncl: collecting pattern correlation for each variable and plotting correlation plot (Fig 9.6)
- ipcc\_ar5/tsline.ncl: time series of the global mean (anomaly) (Fig. 9.8)
- ipcc\_ar5/ch09\_fig09\_14.py: Zonally averaged and equatorial SST (Fig. 9.14)
- seaice/seaice\_tsline.ncl: Time series of sea ice extent (Fig. 9.24a/b)
- seaice/seaice\_trends.ncl: Trend distributions of sea ice extent (Fig 9.24c/d)
- regional\_downscaling/Figure9\_38.ncl (Fig 9.38a (variable tas) and Fig 9.38b (variable pr))
- regional\_downscaling/Figure9\_39.ncl (Fig 9.39a/c/e (variable tas) and Fig 9.39b/d/f (variable pr))
- regional\_downscaling/Figure9\_40.ncl (Fig 9.40a/c/e (variable tas) and Fig 9.40b/d/f (variable pr))
- regional\_downscaling/Figure9\_41.ncl (Fig 9.41b)
- ipcc\_ar5/ch09\_fig09\_42a.py: ECS vs. surface air temperature (Fig. 9.42a)
- ipcc\_ar5/ch09\_fig09\_42b.py: TCR vs. ECS (Fig. 9.42b)
- emergent\_constraints/snowalbedo.ncl: snow-albedo effect (Fig. 9.45a)

# 18.2.3 User settings in recipe

1. Script carbon\_cycle/main.ncl

See *here*.

2. Script climate\_metrics/ecs.py

See *here*.

3. Script clouds/clouds\_bias.ncl

Required settings (scripts)

none

Optional settings (scripts)

- plot\_abs\_diff: additionally also plot absolute differences (true, false)
- plot\_rel\_diff: additionally also plot relative differences (true, false)
- projection: map projection, e.g., Mollweide, Mercator

- timemean: time averaging, i.e. "seasonalclim" (DJF, MAM, JJA, SON), "annualclim" (annual mean)
- Required settings (variables)\*
- reference\_dataset: name of reference dataset

Optional settings (variables)

• long\_name: description of variable

Color tables

- variable "tas": diag\_scripts/shared/plot/rgb/ipcc-tas.rgb, diag\_scripts/shared/plot/rgb/ipcc-tas-delta.rgb
- variable "pr-mmday": diag\_scripts/shared/plots/rgb/ipcc-precip.rgb, diag\_scripts/shared/plot/rgb/ipcc-precip-delta.rgb
- 4. Script clouds/clouds\_ipcc.ncl

Required settings (scripts)

none

Optional settings (scripts)

- explicit\_cn\_levels: contour levels
- mask\_ts\_sea\_ice: true = mask T < 272 K as sea ice (only for variable "ts"); false = no additional grid cells masked for variable "ts"
- projection: map projection, e.g., Mollweide, Mercator
- styleset: style set for zonal mean plot ("CMIP5", "DEFAULT")
- timemean: time averaging, i.e. "seasonalclim" (DJF, MAM, JJA, SON), "annualclim" (annual mean)
- valid\_fraction: used for creating sea ice mask (mask\_ts\_sea\_ice = true): fraction of valid time steps required to mask grid cell as valid data

Required settings (variables)

• reference\_dataset: name of reference data set

Optional settings (variables)

- long\_name: description of variable
- units: variable units

Color tables

- variables "pr", "pr-mmday": diag\_scripts/shared/plot/rgb/ipcc-precip-delta.rgb
- 5. Script ipcc\_ar5/tsline.ncl

Required settings for script

• styleset: as in diag\_scripts/shared/plot/style.ncl functions

Optional settings for script

- time\_avg: type of time average (currently only "yearly" and "monthly" are available).
- ts\_anomaly: calculates anomalies with respect to the defined period; for each grid point by removing the mean for the given calendar month (requiring at least 50% of the data to be non-missing)
- ref\_start: start year of reference period for anomalies
- ref\_end: end year of reference period for anomalies

- ref\_value: if true, right panel with mean values is attached
- ref\_mask: if true, model fields will be masked by reference fields
- region: name of domain
- plot\_units: variable unit for plotting
- y-min: set min of y-axis
- y-max: set max of y-axis
- mean\_nh\_sh: if true, calculate first NH and SH mean
- · volcanoes: if true, lines of main volcanic eruptions will be added
- run\_ave: if not equal 0 than calculate running mean over this number of years
- header: if true, region name as header

Required settings for variables

### none

Optional settings for variables

• reference\_dataset: reference dataset; REQUIRED when calculating anomalies

Color tables

- e.g. diag\_scripts/shared/plot/styles/cmip5.style
- 6. Script ipcc\_ar5/ch09\_fig09\_3.ncl

Required settings for script

none

Optional settings for script

• projection: map projection, e.g., Mollweide, Mercator (default = Robinson)

Required settings for variables

• reference\_dataset: name of reference observation

Optional settings for variables

- map\_diff\_levels: explicit contour levels for plotting
- 7. Script ipcc\_ar5/ch09\_fig09\_6.ncl

Required settings for variables

• reference\_dataset: name of reference observation

Optional settings for variables

- alternative\_dataset: name of alternative observations
- 8. Script ipcc\_ar5/ch09\_fig09\_6\_collect.ncl

Required settings for script

none

Optional settings for script

• diag\_order: List of diagnostic names in the order variables should appear on x-axis

- 9. Script seaice/seaice\_trends.ncl
  - Required settings (scripts)
    - month: selected month (1, 2, ..., 12) or annual mean ("A")
    - region: region to be analyzed ( "Arctic" or "Antarctic")
  - Optional settings (scripts)
    - fill\_pole\_hole: fill observational hole at North pole, Default: False
  - Optional settings (variables)
    - ref\_model: array of references plotted as vertical lines
- 10. Script seaice/seaice\_tsline.ncl

Required settings (scripts)

- region: Arctic, Antarctic
- month: annual mean (A), or month number (3 = March, for Antarctic; 9 = September for Arctic)

Optional settings (scripts)

- styleset: for plot\_type cycle only (cmip5, cmip6, default)
- multi\_model\_mean: plot multi-model mean and standard deviation (default: False)
- EMs\_in\_lg: create a legend label for individual ensemble members (default: False)
- fill\_pole\_hole: fill polar hole (typically in satellite data) with sic = 1 (default: False)
- 11. Script regional\_downscaling/Figure9.38.ncl

Required settings for script

none

Optional settings (scripts)

- styleset: for plot\_type cycle (e.g. CMIP5, CMIP6), default "CMIP5"
- fig938\_region\_label: Labels for regions, which should be included (["WNA", "ENA", "CAM", "TSA", "SSA", "EUM", "NAF", "CAF", "SAF", "NAS", "CAS", "EAS", "SAS", "SEA", "AUS"]), default "WNA"
- fig938\_project\_MMM: projects to average, default "CMIP5"
- fig938\_experiment\_MMM: experiments to average, default "historical"
- fig938\_mip\_MMM: mip to average, default "Amon"
- fig938\_names\_MMM: names in legend i.e. (["CMIP5","CMIP3"]), default fig938\_project\_MMM
- fig938\_colors\_MMM: Color for multi-model mean (e.g. ["red"]), default "red"
- If set fig938\_mip\_MMM, fig938\_experiment\_MMM, fig938\_project\_MMM, fig938\_names\_MMM, and fig938\_colors\_MMM must have the same number of elements
- fig938\_refModel: Reference data set for differences default "ERA-Interim"
- fig938\_MMM: Plot multi-model mean (true/false), default "true"
- fig938\_YMin: minimum Y Axis
- fig938\_YMax: maximum Y Axis
- fig938\_diff: Difference to reference data (true) or absolute annual cycle (false), default "true"

- 12. Script regional\_downscaling/Figure9.39.ncl
  - Required settings (scripts)
    - reference\_dataset: reference dataset name (set of variables)

Optional settings (scripts)

- styleset: for plot\_type cycle (e.g. CMIP5, CMIP6), default "CMIP5"
- fig939\_season: seasons i.e. (["DJF","JJA","ANN"]), default "DJF"
- fig939\_region\_label: Labels for regions, which should be included (["ALAs","CGIs","WNAs","CNAs","ENAs","CAMs","AMZs","NEBs","WSAs","SSAs", "NEUs","CEUs","MEDs","SAHs","WAFs","EAFs","SAFs","NASs","WASs","CASs", "TIBs","EASs","SASs","SASs","SAUs"]), default "ALAs"
- fig939\_project\_MMM: projects to average, default "CMIP5"
- fig939\_experiment\_MMM: experiments to average, default "historical"
- fig939\_mip\_MMM: mip to average, default "Amon"
- fig939\_MMM: Plot multi-model mean (true/false)
- fig939\_names\_MMM: names in legend i.e. (["CMIP5","CMIP3"])
- fig939\_YMin: minimum Y Axis
- fig939\_YMax: maximum Y Axis
- fig939\_vert\_line\_pos: i.e. ([6,10,13,17,24,26])
- fig939\_vert\_line\_label: labels of vertical lines, i.e. (["North America", "South America", "Europe", "Africa", "Asia", "Australia"])
- fig939\_mode: True= cumulative mode
- 13. Script regional\_downscaling/Figure9.40.ncl

Required settings (scripts)

• reference\_dataset: reference dataset name (set of variables)

*Optional settings (scripts)* 

- styleset: for plot\_type cycle (e.g. CMIP5, CMIP6), default "CMIP5"
- fig940\_season: seasons i.e. (["DJF","JJA","ANN"]), default "DJF"
- fig940\_region\_label: Labels for regions, which should be included (["Arc-tic\_land","Arctic\_sea","Antarctic\_land","Antarctic\_sea", "Caribbean","WesternIndianOcean","NorthernIndianOcean", "NorthernTropicalPacific", "SouthernTropicalPacific", "SouthernTropicalPacific", "World\_land","World\_sea","World"]), default "Arctic\_land"
- fig940\_project\_MMM: projects to average, default "CMIP5"
- fig940\_experiment\_MMM: experiments to average, default "historical"
- fig940\_mip\_MMM: mip to average, default "Amon"
- fig940\_MMM: Plot multi-model mean (true/false)
- fig940\_names\_MMM: names in legend i.e. (["CMIP5","CMIP3"])
- fig940\_YMin: minimum Y Axis
- fig940\_YMax: maximum Y Axis

- fig940\_vert\_line\_pos: i.e. ([6,10,13,17,24,26])
- fig940\_vert\_line\_label: labels of vertical lines, i.e. (["North America", "South America", "Europe", "Africa", "Asia", "Australia"])
- fig940\_mode: True= cumulative mode
- 14. Script regional\_downscaling/Figure9.41.ncl

*Required settings (scripts)* 

• reference\_dataset: reference dataset name (set of variables)

Optional settings (scripts)

- styleset: for plot\_type cycle (e.g. CMIP5, CMIP6), default "CMIP5"
- fig941\_region\_label: Labels for regions, which should be included (["ALAs","CGIs","WNAs","CNAs","ENAs","CAMs","AMZs","NEBs","WSAs","SSAs", "NEUs","CEUs","MEDs","SAHs","WAFs","EAFs","SAFs","NASs","WASs","CASs", "TIBs","EASs","SASs","SASs","SASs","SASs","SAUs"]), default "MEDs"
- 15. Script ipcc\_ar5/ch09\_fig09\_42a.py

Required settings for script

none

Optional settings for script

- axes\_functions: dict containing methods executed for the plot's matplotlib.axes.Axes object.
- dataset\_style: name of the style file (located in esmvaltool.diag\_scripts.shared.plot. styles\_python).
- matplotlib\_style: name of the matplotlib style file (located in esmvaltool.diag\_scripts.shared. plot.styles\_python.matplotlib).
- save: dict containing keyword arguments for the function matplotlib.pyplot.savefig().
- seaborn\_settings: Options for seaborn.set\_theme() (affects all plots).
- 1. Script ipcc\_ar5/ch09\_fig09\_42b.py

*Required settings for script* 

none

Optional settings for script

- dataset\_style: Dataset style file (located in esmvaltool.diag\_scripts.shared.plot. styles\_python). The entry marker is ignored when marker\_file is given.
- log\_x: Apply logarithm to X axis (ECS).
- log\_y: Apply logarithm to Y axis (TCR).
- marker\_column: Name of the column to look up markers in marker\_file.
- marker\_file: CSV file with markers (can also be integers). Must have the columns dataset and marker (or the column specified by marker\_column). If a relative path is given, assumes that this is a pattern to search for ancestor files.
- savefig\_kwargs: Keyword arguments for matplotlib.pyplot.savefig().
- seaborn\_settings: Options for seaborn.set\_theme() (affects all plots).
- x\_lim: Plot limits for X axis (ECS).

- y\_lim: Plot limits for Y axis (TCR).
- 2. Script emergent\_constraints/snowalbedo.ncl

Required settings for script

- exp\_presentday: name of present-day experiment (e.g. "historical")
- exp\_future: name of climate change experiment (e.g. "rcp45")

Optional settings for script

- diagminmax: observational uncertainty (min and max)
- legend\_outside: create extra file with legend (true, false)
- styleset: e.g. "CMIP5" (if not set, this diagnostic will create its own color table and symbols for plotting)
- suffix: string to be added to output filenames
- xmax: upper limit of x-axis (default = automatic)
- xmin: lower limit of x-axis (default = automatic)
- ymax: upper limit of y-axis (default = automatic)
- ymin: lower limit of y-axis (default = automatic)

Required settings for variables

• ref\_model: name of reference data set

Optional settings for variables

none

# 18.2.4 Variables

- areacello (fx, longitude latitude)
- fgco2 (ocean, monthly mean, longitude latitude time)
- nbp (ocean, monthly mean, longitude latitude time)
- pr (atmos, monthly mean, longitude latitude time)
- rlut, rlutcs (atmos, monthly mean, longitude latitude time)
- rsdt (atmos, monthly mean, longitude latitude time)
- rsuscs, rsdscs (atmos, monthly mean, longitude latitude time)
- rsut, rsutcs (atmos, monthly mean, longitude latitude time)
- sic (ocean-ice, monthly mean, longitude latitude time)
- tas (atmos, monthly mean, longitude latitude time)
- tos (ocean, monthly mean, longitude, latitude, time)

# 18.2.5 Observations and reformat scripts

Note: (1) obs4MIPs data can be used directly without any preprocessing; (2) see headers of reformat scripts for non-obs4MIPs data for download instructions.

- CERES-EBAF (rlut, rlutcs, rsut, rsutcs obs4MIPs)
- ERA-Interim (tas, ta, ua, va, zg, hus esmvaltool/cmorizers/data/formatters/datasets/era-interim.py)
- GCP2018 (fgco2, nbp esmvaltool/cmorizers/data/formatters/datasets/gcp2018.py)
- GPCP-SG (pr obs4MIPs)
- JMA-TRANSCOM (fgco2, nbp esmvaltool/cmorizers/data/formatters/datasets/jma\_transcom.py)
- HadCRUT4 (tas esmvaltool/cmorizers/data/formatters/datasets/hadcrut4.ncl)
- HadISST (sic, tos esmvaltool/cmorizers/data/formatters/datasets/hadisst.ncl)
- ISCCP-FH (rsuscs, rsdscs, rsdt esmvaltool/cmorizers/data/formatters/datasets/isccp\_fh.ncl)

# 18.2.6 References

- Flato, G., J. Marotzke, B. Abiodun, P. Braconnot, S.C. Chou, W. Collins, P. Cox, F. Driouech, S. Emori, V. Eyring, C. Forest, P. Gleckler, E. Guilyardi, C. Jakob, V. Kattsov, C. Reason and M. Rummukainen, 2013: Evaluation of Climate Models. In: Climate Change 2013: The Physical Science Basis. Contribution of Working Group I to the Fifth Assessment Report of the Intergovernmental Panel on Climate Change [Stocker, T.F., D. Qin, G.-K. Plattner, M. Tignor, S.K. Allen, J. Boschung, A. Nauels, Y. Xia, V. Bex and P.M. Midgley (eds.)]. Cambridge University Press, Cambridge, United Kingdom and New York, NY, USA.
- Hall, A., and X. Qu, 2006: Using the current seasonal cycle to constrain snow albedo feedback in future climate change, Geophys. Res. Lett., 33, L03502, doi:10.1029/2005GL025127.
- Jones et al., 2013: Attribution of observed historical near-surface temperature variations to anthropogenic and natural causes using CMIP5 simulations. Journal of Geophysical Research: Atmosphere, 118, 4001-4024, doi:10.1002/jgrd.50239.
- Seneviratne, S. I., Nicholls, N., Easterling, D., Goodess, C. M., Kanae, S., Kossin, J., Luo, Y., Marengo, J., McInnes, K., Rahimi, M., Reichstein, M., Sorteberg, A., Vera, C., and Zhang, X., 2012: Changes in climate extremes and their impacts on the naturalphysical environment., in: Managing the Risks of Extreme Events and Disasters to Advance Climate Change Adaptation. A Special Report of Working Groups I and II of the Intergovernmental Panel on ClimateChange (IPCC), edited by: Field, C. B., Barros, V., Stocker, T. F., Qin, D., Dokken, D. J., Ebi, K. L., Mastrandrea, M. D., Mach, K. J., Plattner, G.-K., Allen, S. K., Tignor, M., and Midgley, P. M., Cambridge University Press, Cambridge, UK, and New York, NY, USA, 109-230.
- Weigel, K., Bock, L., Gier, B. K., Lauer, A., Righi, M., Schlund, M., Adeniyi, K., Andela, B., Arnone, E., Berg, P., Caron, L.-P., Cionni, I., Corti, S., Drost, N., Hunter, A., Lledó, L., Mohr, C. W., Paçal, A., Pérez-Zanón, N., Predoi, V., Sandstad, M., Sillmann, J., Sterl, A., Vegas-Regidor, J., von Hardenberg, J., and Eyring, V.: Earth System Model Evaluation Tool (ESMValTool) v2.0 - diagnostics for extreme events, regional and impact evaluation, and analysis of Earth system models in CMIP, Geosci. Model Dev., 14, 3159-3184, https: //doi.org/10.5194/gmd-14-3159-2021, 2021.

# 18.2.7 Example plots

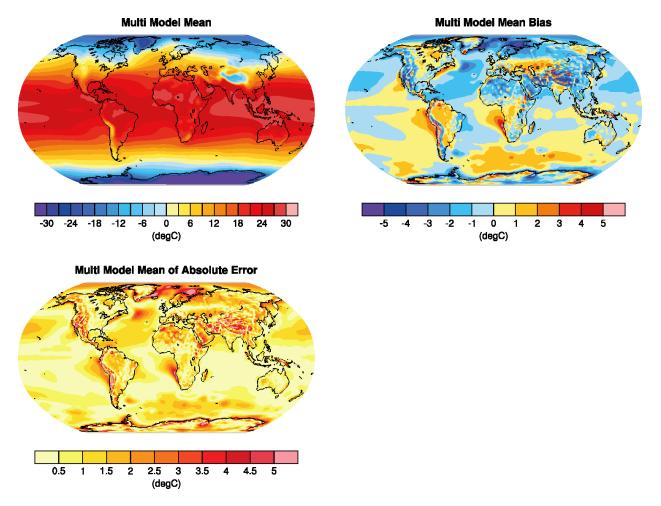


Fig. 11: Figure 9.2 a,b,c: Annual-mean surface air temperature for the period 1980-2005. a) multi-model mean, b) bias as the difference between the CMIP5 multi-model mean and the climatology from ERA-Interim (Dee et al., 2011), c) mean absolute model error with respect to the climatology from ERA-Interim.

# 18.3 IPCC AR5 Chapter 12 (selected figures)

# 18.3.1 Overview

The goal is to create a standard recipe for creating selected Figures from IPCC AR5 Chapter 12 on "Long-term Climate Change: Projections, Commitments and Irreversibility". These include figures showing the change in a variable between historical and future periods, e.g. maps (2D variables), zonal means (3D variables), timeseries showing the change in certain variables from historical to future periods for multiple scenarios, and maps visualizing change in variables normalized by global mean temperature change (pattern scaling) as in Collins et al., 2013.

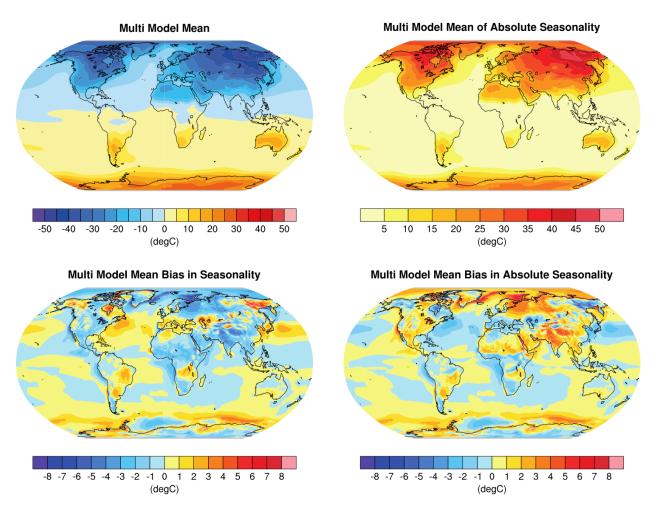


Fig. 12: Figure 9.3: Multi model values for seasonality of near-surface temperature, from top left to bottom right: mean, mean of absolute seasonality, mean bias in seasonality, mean bias in absolute seasonality. Reference dataset: ERA-Interim.

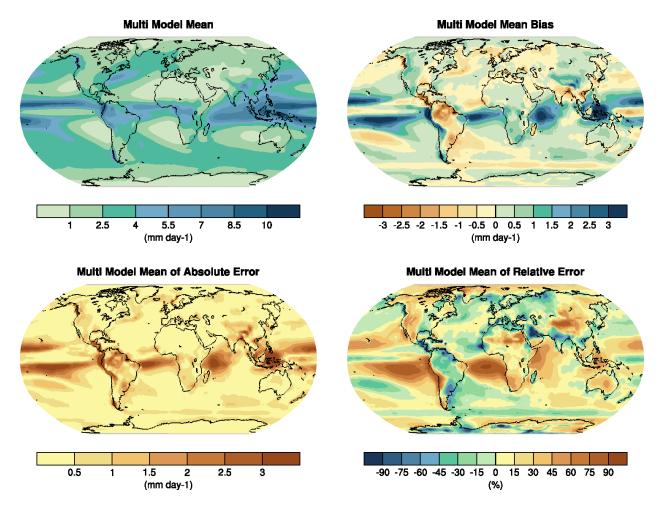


Fig. 13: Figure 9.4: Annual-mean precipitation rate (mm day-1) for the period 1980-2005. a) multi-model mean, b) bias as the difference between the CMIP5 multi-model mean and the climatology from the Global Precipitation Climatology Project (Adler et al., 2003), c) multi-model mean absolute error with respect to observations, and d) multi-model mean error relative to the multi-model mean precipitation itself.

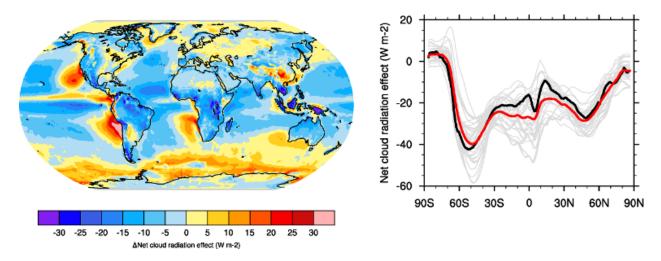


Fig. 14: Figure 9.5: Climatological (1985-2005) annual-mean cloud radiative effects in Wm-2 for the CMIP5 models against CERES EBAF (2001-2011) in Wm-2. Top row shows the shortwave effect; middle row the longwave effect, and bottom row the net effect. Multi-model-mean biases against CERES EBAF 2.6 are shown on the left, whereas the right panels show zonal averages from CERES EBAF 2.6 (black), the individual CMIP5 models (thin gray lines), and the multi-model mean (thick red line).

# 18.3.2 Available recipes and diagnostics

Recipes are stored in recipes/

• recipe\_collins13ipcc.yml

Diagnostics are stored in diag\_scripts/

- ipcc\_ar5/ch12\_map\_diff\_each\_model\_fig12-9.ncl: calculates the difference between future and historical runs for one scenario for each given model individually on their native grid and plots all of them in one Figure. As in Figure 12.9 in AR5.
- ipcc\_ar5/ch12\_ts\_line\_mean\_spread.ncl: calculates time series for one variable, change in future relative to base period in historical, multi-model mean as well as spread around it (as standard deviation).
- ipcc\_ar5/ch12\_plot\_ts\_line\_mean\_spread.ncl: plots the timeseries multi-model mean and spread calculated above. As in Figure 12.5 in AR5.
- ipcc\_ar5/ch12\_calc\_IAV\_for\_stippandhatch.ncl: calculates the interannual variability over piControl runs, either over the whole time period or in chunks over some years.
- ipcc\_ar5/ch12\_calc\_map\_diff\_mmm\_stippandhatch.ncl: calculates the difference between future and historical periods for each given model and then calculates multi-model mean as well as significance. Significant is where the multi-model mean change is greater than two standard deviations of the internal variability and where at least 90% of the models agree on the sign of change. Not significant is where the multi-model mean change is less than one standard deviation of internal variability.
- ipcc\_ar5/ch12\_plot\_map\_diff\_mmm\_stipp.ncl: plots multi-model mean maps calculated above including stippling where significant and hatching where not significant. As in Figure 12.11 in AR5.
- ipcc\_ar5/ch12\_calc\_zonal\_cont\_diff\_mmm\_stippandhatch.ncl: calculates zonal means and the difference between future and historical periods for each given model and then calculates multi-model mean as well as significance as above.
- ipcc\_ar5/ch12\_plot\_zonal\_diff\_mmm\_stipp.ncl: plots the multi-model mean zonal plots calculated above including stippling where significant and hatching where not significant. As in Figure 12.12 in AR5.

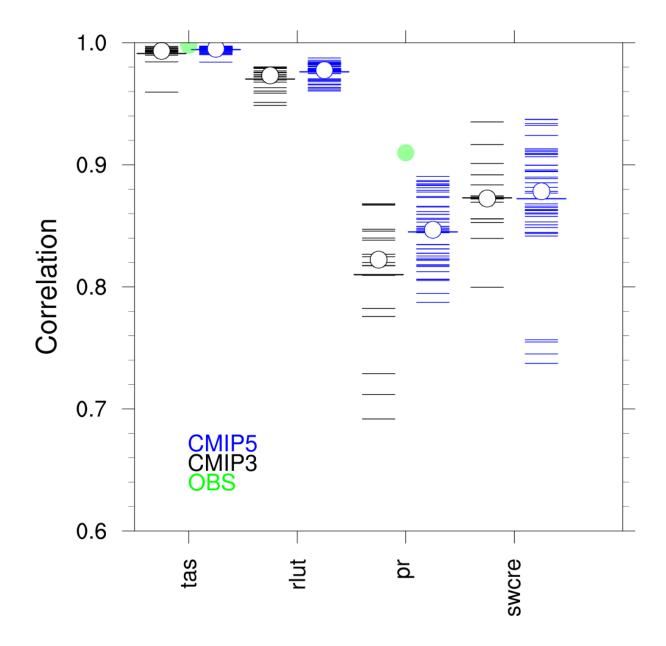


Fig. 15: Figure 9.6: Centered pattern correlations between models and observations for the annual mean climatology over the period 1980–1999. Results are shown for individual CMIP3 (black) and CMIP5 (blue) models as thin dashes, along with the corresponding ensemble average (thick dash) and median (open circle). The four variables shown are surface air temperature (TAS), top of the atmosphere (TOA) outgoing longwave radiation (RLUT), precipitation (PR) and TOA shortwave cloud radiative effect (SW CRE). The correlations between the reference and alternate observations are also shown (solid green circles).

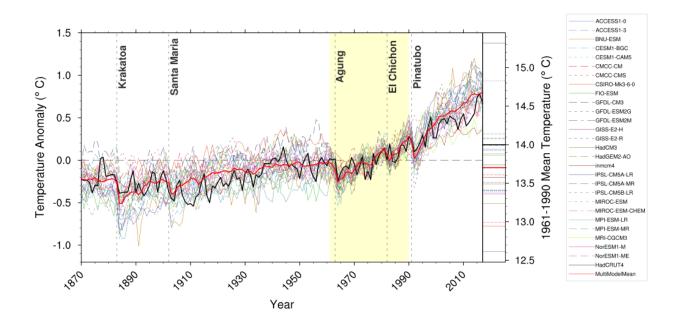


Fig. 16: Figure 9.8: Observed and simulated time series of the anomalies in annual and global mean surface temperature. All anomalies are differences from the 1961-1990 time-mean of each individual time series. The reference period 1961-1990 is indicated by yellow shading; vertical dashed grey lines represent times of major volcanic eruptions. Single simulations for CMIP5 models (thin lines); multi-model mean (thick red line); different observations (thick black lines). Dataset pre-processing like described in Jones et al., 2013.

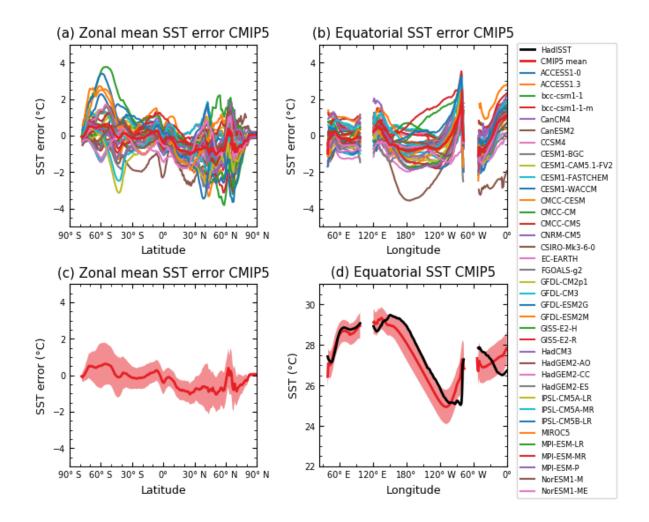


Fig. 17: Figure 9.14: (a) Zonally averaged sea surface temperature (SST) error in CMIP5 models. (b) Equatorial SST error in CMIP5 models. (c) Zonally averaged multi-model mean SST error for CMIP5 together with inter-model standard deviation (shading). (d) Equatorial multi-model mean SST in CMIP5 together with inter-model standard deviation (shading) and observations (black). Model climatologies are derived from the 1979-1999 mean of the historical simulations. The Hadley Centre Sea Ice and Sea Surface Temperature (HadISST) (Rayner et al., 2003) observational climatology for 1979-1999 is used as a reference for the error calculation (a), (b), and (c); and for observations in (d).

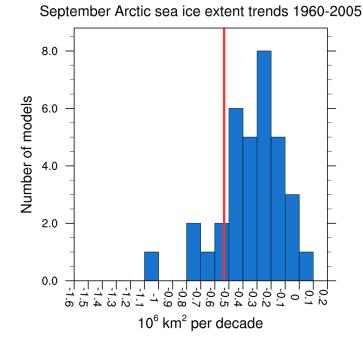


Fig. 18: Figure 9.24c: Sea ice extent trend distribution for the Arctic in September.

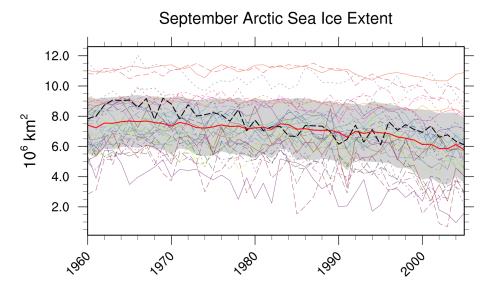


Fig. 19: Figure 9.24a: Time series of total sea ice area and extent (accumulated) for the Arctic in September including multi-model mean and standard deviation.

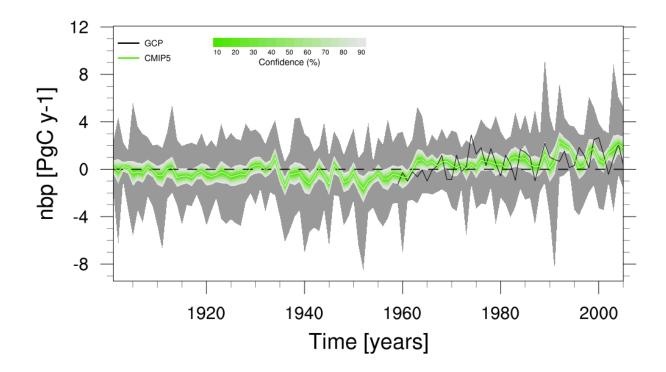


Fig. 20: Figure 9.26 (bottom): Ensemble-mean global land carbon uptake in the CMIP5 ESMs for the historical period 1900–2005. For comparison, the observation-based estimates provided by the Global Carbon Project (GCP) are also shown (black line). The confidence limits on the ensemble mean are derived by assuming that the CMIP5 models come from a t-distribution. The grey areas show the range of annual mean fluxes simulated across the model ensemble.

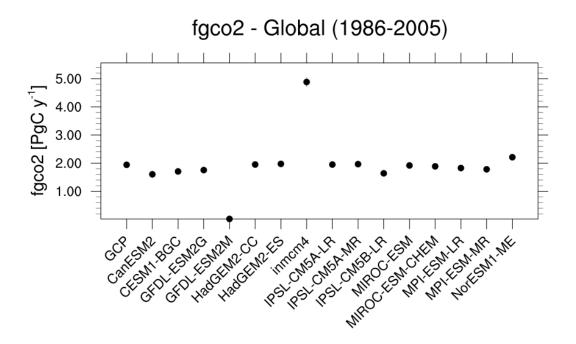


Fig. 21: Figure 9.27 (top): Simulation of global mean atmosphere–ocean CO2 fluxes ("fgCO2") by ESMs for the period 1986–2005. For comparison, the observation-based estimates provided by Global Carbon Project (GCP) are also shown. The error bars for the ESMs and observations represent interannual variability in the fluxes, calculated as the standard deviation of the annual means over the period 1986–2005.

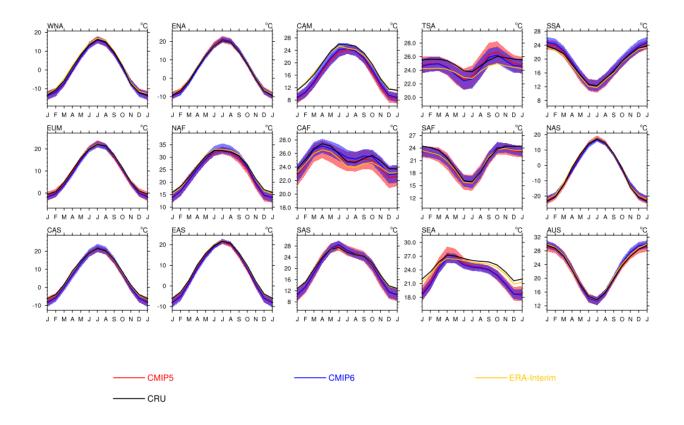


Fig. 22: Figure 9.38tas: Mean seasonal cycle for surface temperature (tas) as multi model mean of 38 CMIP5 and 22 CMIP6 models as well as CRU and ERA-Interim reanalysis data averaged for 1980-2005 over land in different regions: Western North America (WNA), Eastern North America (ENA), Central America (CAM), Tropical South America (TSA), Southern South America (SSA), Europe and Mediterranean (EUM), North Africa (NAF), Central Africa (CAF), South Africa (SAF), North Asia (NAS), Central Asia (CAS), East Asia (EAS), South Asia (SAS), Southeast Asia (SEA), and Australia (AUS). Similar to Fig. 9.38a from Flato et al. (2013), CMIP6 instead of CMIP3 and set of CMIP5 models used different.

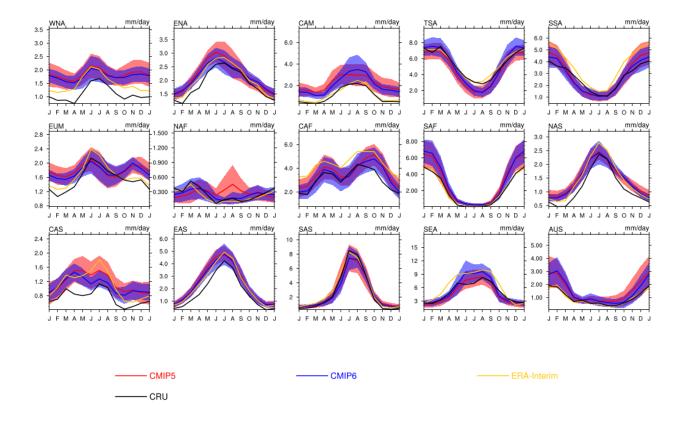


Fig. 23: Figure 9.38pr: Mean seasonal cycle for precipitation (pr) as multi model mean of 38 CMIP5 and 22 CMIP6 models as well as CRU and ERA-Interim reanalysis data averaged for 1980-1999 over land in different regions: Western North America (WNA), Eastern North America (ENA), Central America (CAM), Tropical South America (TSA), Southern South America (SSA), Europe and Mediterranean (EUM), North Africa (NAF), Central Africa (CAF), South Africa (SAF), North Asia (NAS), Central Asia (CAS), East Asia (EAS), South Asia (SAS), Southeast Asia (SEA), and Australia (AUS). Similar to Fig. 9.38b from Flato et al. (2013), CMIP6 instead of CMIP3 and set of CMIP5 models used different.

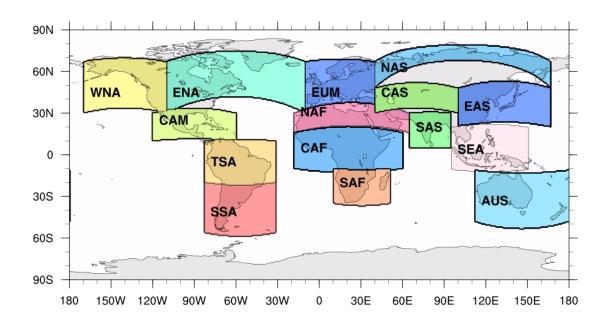
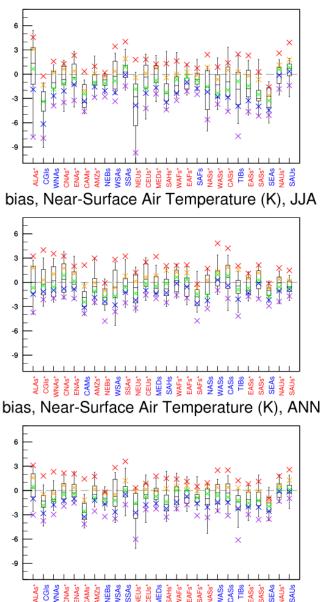


Fig. 24: Figure 9.38reg: Positions of the regions used in Figure 9.38.



bias, Near-Surface Air Temperature (K), DJF

Fig. 25: Figure 9.39tas: Box and whisker plots showing the 5th, 25th, 50th, 75th and 95th percentiles of the seasonal- and annual mean biases for surface temperature (tas) for 1980-2005 between 38 CMIP5 models (box and whiskers) or 22 CMIP6 models (crosses) and CRU data. The regions are: Alaska/NW Canada (ALAs), Eastern Canada/Greenland/Iceland (CGIs), Western North America(WNAs), Central North America (CNAs), Eastern North America (ENAs), Central America/Mexico (CAMs), Amazon (AMZs), NE Brazil (NEBs), West Coast South America (WSAs), South-Eastern South America (SSAs), Northern Europe (NEUs), Central Europe (CEUs), Southern Europe/the Mediterranean (MEDs), Sahara (SAHs), Western Africa (WAFs), Eastern Africa (EAFs), Southern Africa (SAFs), Northern Asia (NASs), Western Asia (WASs), Central Asia (CASs), Tibetan Plateau (TIBs), Eastern Asia (EASs), Southern Asia (SASs), Southeast Asia (SEAs), Northern Australia (NASs) and Southern Australia/New Zealand (SAUs). The positions of these regions are defined following (Seneviratne et al., 2012) and differ from the ones in Fig. 9.38. Similar to Fig. 9.39 a,c,e from Flato et al. (2013), CMIP6 instead of CMIP3 and set of CMIP5 models used different.

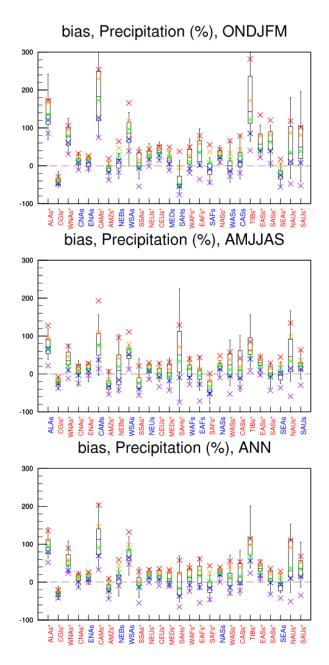


Fig. 26: Figure 9.39pr: Box and whisker plots showing the 5th, 25th, 50th, 75th and 95th percentiles of the seasonal- and annual mean biases for precipitation (pr) for 1980-2005 between 38 CMIP5 models (box and whiskers) or 22 CMIP6 models (crosses) and CRU data. The regions are: Alaska/NW Canada (ALAs), Eastern Canada/Greenland/Iceland (CGIs), Western North America(WNAs), Central North America (CNAs), Eastern North America (ENAs), Central America/Mexico (CAMs), Amazon (AMZs), NE Brazil (NEBs), West Coast South America (WSAs), South-Eastern South America (SSAs), Northern Europe (NEUs), Central Europe (CEUs), Southern Europe/the Mediterranean (MEDs), Sahara (SAHs), Western Africa (WAFs), Eastern Africa (EAFs), Southern Africa (SAFs), Northern Asia (NASs), Western Asia (SASs), Central Asia (CASs), Tibetan Plateau (TIBs), Eastern Asia (EASs), Southern Asia (SASs), Southern Australia (NASs) and Southern Australia/New Zealand (SAUs). The positions of these regions are defined following (Seneviratne et al., 2012) and differ from the ones in Fig. 9.38. Similar to Fig. 9.39 b,d,f from Flato et al. (2013), CMIP6 instead of CMIP3 and set of CMIP5 models used different.

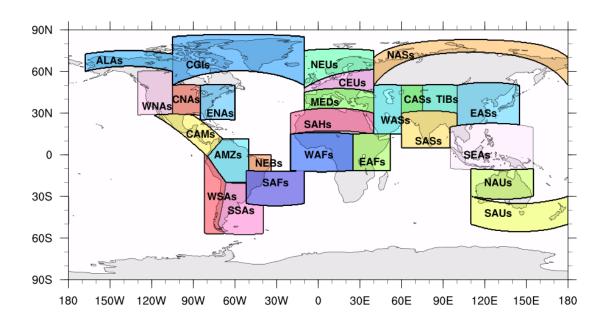
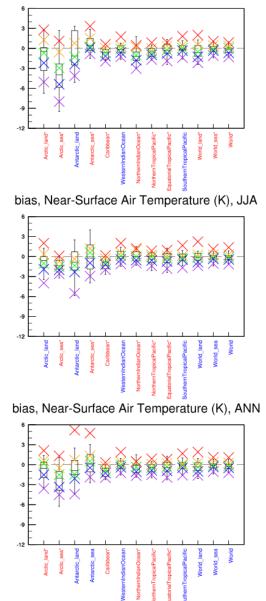


Fig. 27: Figure 9.39reg: Positions of the regions used in Figure 9.39.



bias, Near-Surface Air Temperature (K), DJF

Fig. 28: Figure 9.40tas: Box and whisker plots showing the 5th, 25th, 50th, 75th and 95th percentiles of the seasonaland annual mean biases for surface temperature (tas) for oceanic and polar regions between 38 CMIP5 (box and whiskers) or 22 CMIP6 (crosses) models and ERA-Interim data for 1980–2005.

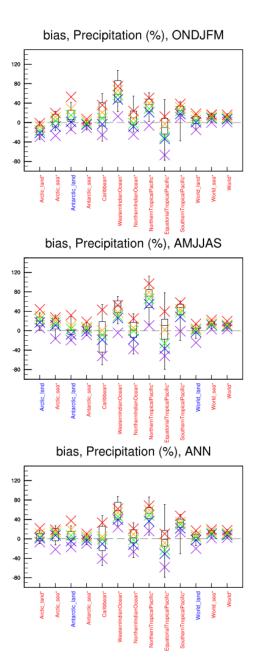


Fig. 29: Figure 9.40pr: Box and whisker plots showing the 5th, 25th, 50th, 75th and 95th percentiles of the seasonaland annual mean biases for precipitation (pr) for oceanic and polar regions between 38 CMIP5 (box and whiskers) or 22 CMIP6 (crosses) models and Global Precipitation Climatology Project - Satellite-Gauge (GPCP-SG) data for 1980–2005.

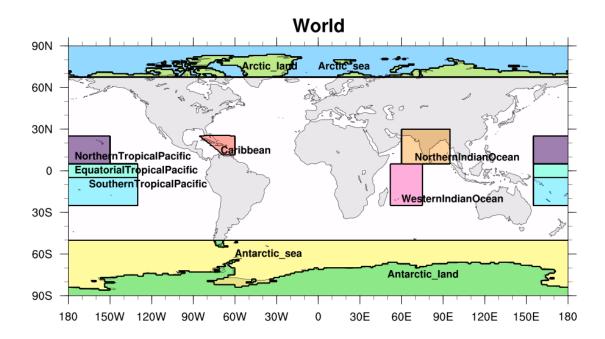


Fig. 30: Figure 9.40reg: Positions of the regions used in Figure 9.40.

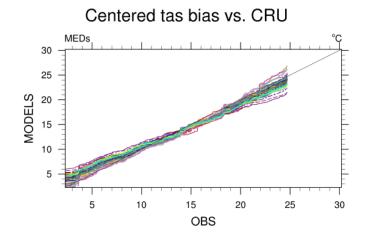


Fig. 31: Figure 9.41b: Ranked modelled versus ERA-Interim mean temperature for 38 CMIP5 models in the Mediterranean region for 1961–2000.

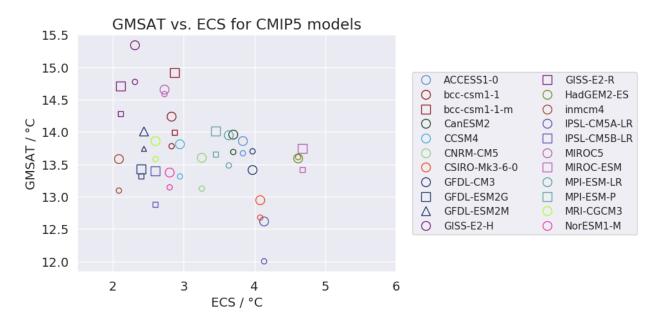


Fig. 32: Figure 9.42a: Equilibrium climate sensitivity (ECS) against the global mean surface air temperature of CMIP5 models, both for the period 1961-1990 (larger symbols) and for the pre-industrial control runs (smaller symbols).

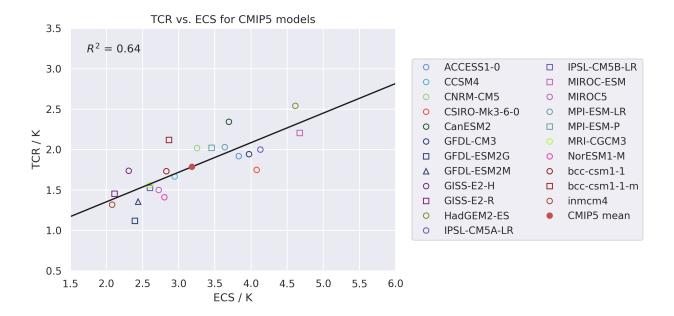


Fig. 33: Figure 9.42b: Transient climate response (TCR) against equilibrium climate sensitivity (ECS) for CMIP5 models.

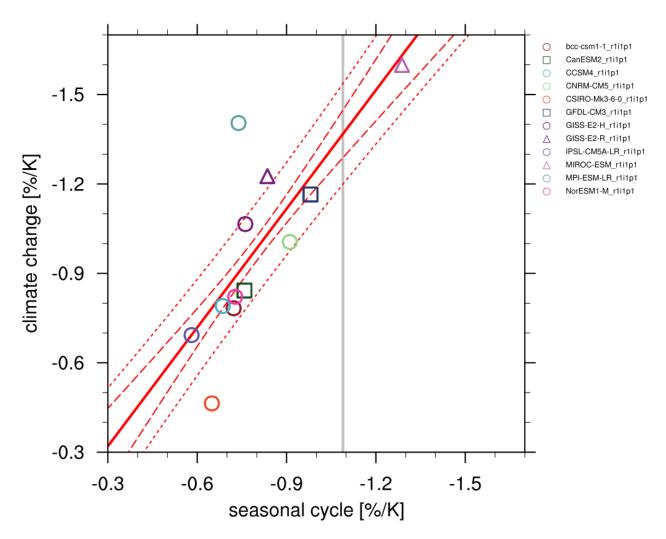


Fig. 34: Figure 9.45a: Scatterplot of springtime snow-albedo effect values in climate change vs. springtime  $\Delta \alpha_s / \Delta T_s$  values in the seasonal cycle in transient climate change experiments (CMIP5 historical experiments: 1901-2000, RCP4.5 experiments: 2101-2200).

- ipcc\_ar5/ch12\_calc\_map\_diff\_scaleT\_mmm\_stipp.ncl: calculates the change in variable between future and historical period normalized by gloabl mean temperature change of each given model and scenario. Then averages over all realizations and calculates significance. Significant is where the mean change averaged over all realizations is larger than the 95% percentile of the distribution of models (assumed to be gaussian). Can be plotted using ipcc\_ar5/ch12\_plot\_map\_diff\_mmm\_stipp.ncl.
- seaice/seaice\_ecs.ncl: scatter plot of historical trend in September Arctic sea ice extent (SSIE) vs historical long-term mean SSIE (similar to Fig. 12.31a in AR5) and historical SSIE trend vs YOD RCP8.5 (similar to Fig. 12.31d in AR5).
- seaice/seaice\_yod.ncl: calculation of year of near disappearance of Arctic sea ice (similar to Fig 12.31e in AR5)
- ipcc\_ar5/ch12\_snw\_area\_change\_fig12-32.ncl: calculate snow area extent in a region (e.g Northern Hemisphere) and season (e.g. Northern Hemisphere spring March & April) relative to a reference period (e.g 1986-2005) and spread over models as in Fig. 12.32 of IPCC AR5. Can be plotted using ipcc\_ar5/ch12\_plot\_ts\_line\_mean\_spread.ncl.

# 18.3.3 User settings

1. Script ipcc\_ar5/ch12\_map\_diff\_each\_model\_fig12-9.ncl

Required settings (script)

- time\_avg: time averaging ("annualclim", "seasonalclim")
- experiment: IPCC Scenario, used to pair historical and rcp runs from same model

Optional settings (script)

- projection: map projection, any valid ncl projection, default = Robinson
- max\_vert: maximum number of plots in vertical
- max\_hori: maximum number of plots in horizontal
- title: plot title
- colormap: alternative colormap, path to rgb file or ncl name
- diff\_levs: list with contour levels for plots
- span: span whole colormap? (True, False, default = False)

*Required settings (variables)* 

- project: CMIP5 (or CMIP6)
- mip: variable mip, generally Amon or Omon
- 2. Script ipcc\_ar5/ch12\_ts\_line\_mean\_spread.ncl

Required settings (script)

- · scenarios: list with scenarios included in figure
- syears: list with start years in time periods (e.g. start of historical period and rcps)
- eyears: list with end years in time periods (end year of historical runs and rcps)
- begin\_ref\_year: start year of reference period (e.g. 1986)
- end\_ref\_year: end year of reference period (e.g 2005)
- label: list with labels to use in legend depending on scenarios

*Optional settings (script)* 

- spread: how many standard deviations to calculate the spread with? default is 1., ipcc tas used 1.64
- model\_nr: save number of model runs per period and scenario in netcdf to print in plot? (True, False, default = False)
- ts\_minlat: minimum latitude if not global
- ts\_maxlat: maximum latitude if not global
- ts\_minlon: minimum longitude if not global
- ts\_maxlon: maximum longitude if not global

Required settings (variables)

- project: CMIP5 (or CMIP6)
- mip: variable mip, generally Amon or Omon
- 3. Script ipcc\_ar5/ch12\_plot\_ts\_line\_mean\_spread.ncl:

Required settings (script)

• ancestors: variable and diagnostics that calculated data to be plotted

Optional settings (script)

- title: specify plot title
- yaxis: specify y-axis title
- ymin: minimim value on y-axis, default calculated from data
- ymax: maximum value on y-axis
- colormap: alternative colormap, path to rgb file or ncl name
- 1. Script ipcc\_ar5/ch12\_calc\_IAV\_for\_stippandhatch.ncl:

#### Required settings (script)

• time\_avg: time averaging ("annualclim", "seasonalclim"), needs to be consistent with calculation in ch12\_calc\_map\_diff\_mmm\_stippandhatch.ncl

Optional settings (script)

- periodlength: length of period in years to calculate variability over, default is total time period
- iavmode: calculate IAV from multi-model mean or save individual models ("each": save individual models, "mmm": multi-model mean, default), needs to be consistent with ch12\_calc\_map\_diff\_mmm\_stippandhatch.ncl

#### Required settings (variables)

- project: CMIP5 (or CMIP6)
- mip: variable mip, generally Amon or Omon
- exp: piControl
- preprocessor: which preprocessor to use, depends on dimension of variable, for 2D preprocessor only needs to regrid, for 3D we need to extract levels either based on reference\_dataset or specify levels.

#### Optional settings (variables)

- reference\_dataset: the reference dataset for level extraction in case of 3D variables.
- 2. Script ipcc\_ar5/ch12\_calc\_map\_diff\_mmm\_stippandhatch.ncl:

Required settings (script)

- ancestors: variable and diagnostics that calculated interannual variability for stippling and hatching
- time\_avg: time averaging ("annualclim", "seasonalclim")
- scenarios: list with scenarios to be included
- periods: list with start years of periods to be included
- label: list with labels to use in legend depending on scenarios

### Optional settings (script)

- seasons: list with seasons index if time\_avg "seasonalclim" (then required), DJF:0, MAM:1, JJA:2, SON:3
- iavmode: calculate IAV from multi-model mean or save individual models ("each": save individual models, "mmm": multi-model mean, default), needs to be consistent with ch12\_calc\_IAV\_for\_stippandhatch.ncl
- percent: determines if difference expressed in percent (0, 1, default = 0)

Required settings (variables)

- project: CMIP5 (or CMIP6)
- mip: variable mip, generally Amon or Omon
- preprocessor: which preprocessor to use, preprocessor only needs to regrid
- 3. Script ipcc\_ar5/ch12\_plot\_map\_diff\_mmm\_stipp.ncl:

### Required settings (script)

• ancestors: variable and diagnostics that calculated field to be plotted

### Optional settings (script)

- projection: map projection, any valid ncl projection, default = Robinson
- diff\_levs: list with explicit levels for all contour plots
- max\_vert: maximum number of plots in vertical
- max\_hori: maximum number of plots in horizontal
- model\_nr: save number of model runs per period and scenario in netcdf to print in plot? (True, False, default = False)
- colormap: alternative colormap, path to rgb file or ncl name
- span: span whole colormap? (True, False, default = True)
- sig: plot stippling for significance? (True, False)
- not\_sig: plot hatching for uncertainty? (True, False)
- pltname: alternative name for output plot, default is diagnostic + varname + time\_avg
- units: units written next to colorbar, e.g (~F35~J~F~C)
- 4. Script ipcc\_ar5/ch12\_calc\_zonal\_cont\_diff\_mmm\_stippandhatch.ncl:

### Required settings (script)

- ancestors: variable and diagnostics that calculated interannual variability for stippling and hatching
- time\_avg: time averaging ("annualclim", "seasonalclim")
- scenarios: list with scenarios to be included
- periods: list with start years of periods to be included
- label: list with labels to use in legend depending on scenarios

*Optional settings (script)* 

- base\_cn: if want contours of base period as contour lines, need to save base period field (True, False)
- seasons: list with seasons index if time\_avg "seasonalclim" (then required), DJF:0, MAM:1, JJA:2, SON:3
- iavmode: calculate IAV from multi-model mean or save individual models ("each": save individual models, "mmm": multi-model mean, default), needs to be consistent with ch12\_calc\_IAV\_for\_stippandhatch.ncl
- percent: determines if difference expressed in percent (0, 1, default = 0)

Required settings (variables)

- project: CMIP5 (or CMIP6)
- mip: variable mip, generally Amon or Omon
- preprocessor: which preprocessor to use, preprocessor needs to regrid, extract leves and calculate the zonal mean.

Optional settings (variables)

- reference\_dataset: the reference dataset for level extraction
- 5. Script ipcc\_ar5/ch12\_plot\_zonal\_diff\_mmm\_stipp.ncl:

Required settings (script)

• ancestors: variable and diagnostics that calculated field to be plotted

Optional settings (script)

- diff\_levs: list with explicit levels for all contour plots
- max\_vert: maximum number of plots in vertical
- max\_hori: maximum number of plots in horizontal
- model\_nr: save number of model runs per period and scenario in netcdf to print in plot? (True, False, default = False)
- colormap: alternative colormap, path to rgb file or ncl name
- span: span whole colormap? (True, False, default = True)
- sig: plot stippling for significance? (True, False)
- not\_sig: plot hatching for uncertainty? (True, False)
- pltname: alternative name for output plot, default is diagnostic + varname + time\_avg
- units: units written next to colorbar in ncl strings, e.g (m s~S~-1~N~)
- if base\_cn: True in ch12\_calc\_zonal\_cont\_diff\_mmm\_stippandhatch.ncl further settings to control contour lines:
  - base\_cnLevelSpacing: spacing between contour levels
  - base\_cnMinLevel: minimum contour line
  - base\_cnMaxLevel: maximum contour line
- 6. Script ipcc\_ar5/ch12\_calc\_map\_diff\_scaleT\_mmm\_stipp.ncl:

Required settings (script)

- time\_avg: time averaging ("annualclim", "seasonalclim")
- scenarios: list with scenarios to be included

- periods: list with start years of periods to be included
- label: list with labels to use in legend depending on scenarios

#### Optional settings (script)

- seasons: list with seasons index if time\_avg "seasonalclim" (then required), DJF:0, MAM:1, JJA:2, SON:3
- percent: determines if difference expressed in percent (0, 1, default = 0)

Required settings (variables)

- project: CMIP5 (or CMIP6)
- mip: variable mip, generally Amon or Omon
- preprocessor: which preprocessor to use, preprocessor only needs to regrid
- 7. Script ipcc\_ar5/ch12\_snw\_area\_change\_fig12-32.ncl:

#### Required settings (script)

- scenarios: list with scenarios included in figure
- syears: list with start years in time periods (e.g. start of historical period and rcps)
- eyears: list with end years in time periods (end year of historical runs and rcps)
- begin\_ref\_year: start year of reference period (e.g. 1986)
- end\_ref\_year: end year of reference period (e.g 2005)
- months: first letters of months included in analysis? e.g. for MA (March + April) for Northern Hemisphere
- label: list with labels to use in legend depending on scenarios

#### Optional settings (script)

- spread: how many standard deviations to calculate the spread with? default is 1., ipcc tas used 1.64
- model\_nr: save number of model runs per period and scenario in netcdf to print in plot? (True, False, default = False)
- colormap: alternative colormap, path to rgb file or ncl name
- ts\_minlat: minimum latitude if not global
- ts\_maxlat: maximum latitude if not global
- ts\_minlon: minimum longitude if not global
- ts\_maxlon: maximum longitude if not global

#### Required settings (variables)

- project: CMIP5 (or CMIP6)
- mip: variable mip, LImon
- fx\_files: [sftlf, sftgif]
- 8. Script seaice/seaice\_ecs.ncl

#### Required settings (scripts)

- hist\_exp: name of historical experiment (string)
- month: selected month (1, 2, ..., 12) or annual mean ("A")
- rcp\_exp: name of RCP experiment (string)

- region: region to be analyzed ( "Arctic" or "Antarctic")
- Optional settings (scripts)
  - fill\_pole\_hole: fill observational hole at North pole (default: False)
  - styleset: color style (e.g. "CMIP5")

Optional settings (variables)

- reference\_dataset: reference dataset
- 9. Script seaice/seaice\_yod.ncl

Required settings (scripts)

- month: selected month (1, 2, ..., 12) or annual mean ("A")
- region: region to be analyzed ( "Arctic" or "Antarctic")

**Optional settings (scripts)** 

- fill\_pole\_hole: fill observational hole at North pole, Default: False
- wgt\_file: netCDF containing pre-determined model weights

Optional settings (variables)

• ref\_model: array of references plotted as vertical lines

### 18.3.4 Variables

Note: These are the variables tested and used in IPCC AR5. However, the code is flexible and in theory other variables of the same kind can be used.

- areacello (fx, longitude latitude)
- clt (atmos, monthly mean, longitude latitude time)
- evspsbl (atmos, monthly mean, longitude latitude time)
- hurs (atmos, monthly mean, longitude latitude time)
- mrro (land, monthly mean, longitude latitude time)
- mrsos (land, monthly mean, longitude latitude time)
- pr (atmos, monthly mean, longitude latitude time)
- psl (atmos, monthly mean, longitude latitude time)
- rlut, rsut, rtmt (atmos, monthly mean, longitude latitude time)
- sic (ocean-ice, monthly mean, longitude latitude time)
- snw (land, monthly mean, longitude latitude time)
- sos (ocean, monthly mean, longitude latitude time)
- ta (atmos, monthly mean, longitude latitude lev time)
- tas (atmos, monthly mean, longitude latitude time)
- thetao (ocean, monthly mean, longitude latitude lev time)
- ua (atmos, monthly mean, longitude latitude lev time)

### 18.3.5 Observations and reformat scripts

• HadISST (sic - esmvaltool/cmorizers/data/formatters/datasets/hadisst.ncl)

### 18.3.6 Reference

Collins, M., R. Knutti, J. Arblaster, J.-L. Dufresne, T. Fichefet, P. Friedlingstein, X. Gao, W.J. Gutowski, T. Johns, G. Krinner, M. Shongwe, C. Tebaldi, A.J. Weaver and M. Wehner, 2013: Long-term Climate Change: Projections, Commitments and Irreversibility. In: Climate Change 2013: The Physical Science Basis. Contribution of Working Group I to the Fifth Assessment Report of the Intergovernmental Panel on Climate Change [Stocker, T.F., D. Qin, G.-K. Plattner, M. Tignor, S.K. Allen, J. Boschung, A. Nauels, Y. Xia, V. Bex and P.M. Midgley (eds.)]. Cambridge University Press, Cambridge, United Kingdom and New York, NY, USA.

## 18.3.7 Example plots

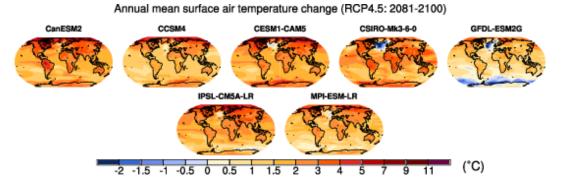


Fig. 35: Surface air temperature change in 2081–2100 displayed as anomalies with respect to 1986–2005 for RCP4.5 from individual CMIP5 models.

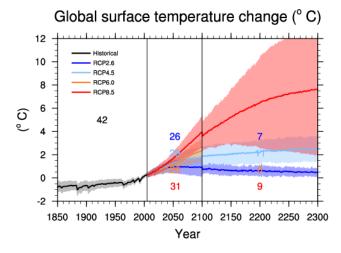
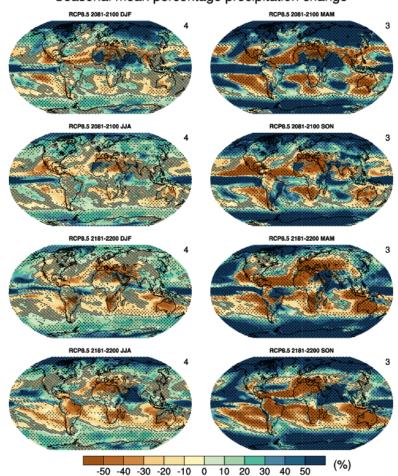


Fig. 36: Time series of global annual mean surface air temperature anomalie (relative to 1986–2005) from CMIP5 concentration-driven experiments.



Seasonal mean percentage precipitation change

Fig. 37: Multi-model CMIP5 average percentage change in seasonal mean precipitation relative to the reference period 1986–2005 averaged over the periods 2081–2100 and 2181–2200 under the RCP8.5 forcing scenario. Hatching indicates regions where the multi-model mean change is less than one standard deviation of internal variability. Stippling indicates regions where the multi-model mean change is greater than two standard deviations of internal variability and where at least 90% of models agree on the sign of change

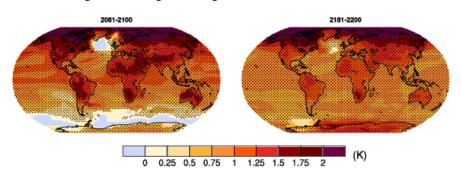


Fig. 38: Temperature change patterns scaled to 1°C of global mean surface temperature change.

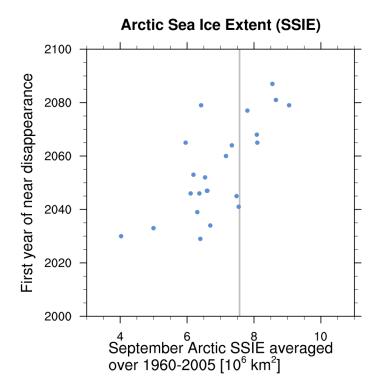


Fig. 39: Scatter plot of mean historical September Arctic sea ice extent vs 1st year of disappearance (RCP8.5) (similar to IPCC AR5 Chapter 12, Fig. 12.31a).

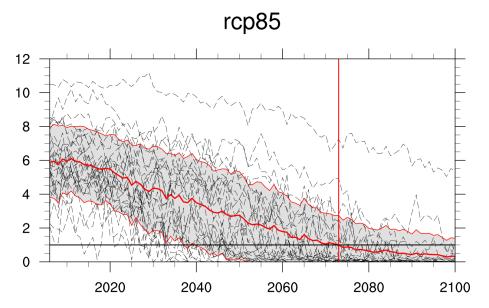


Fig. 40: Time series of September Arctic sea ice extent for individual CMIP5 models, multi-model mean and multimodel standard deviation, year of disappearance (similar to IPCC AR5 Chapter 12, Fig. 12.31e).

# **18.4 Example recipes**

### 18.4.1 Overview

These are example recipes calling example diagnostic scripts.

The recipe examples/recipe\_python.yml produces time series plots of global mean temperature and for the temperature in Amsterdam. It also produces a map of global temperature in January 2020.

The recipe examples/recipe\_easy\_ipcc.yml reproduces part of figure 9.3a from IPCC AR6 - Climate Change 2021: The Physical Science Basis. It demonstrates how ESMValTool can be used to conveniently analyze many models on their native grid and is described in detail in the blog post Analysis-ready climate data with ESMValCore.

The recipe examples/recipe\_extract\_shape.yml produces a map of the mean temperature in the Elbe catchment over the years 2000 to 2002. Some example shapefiles for use with this recipe are available here, make sure to download all files with the same name but different extensions.

The recipe examples/recipe\_julia.yml produces a map plot with the mean temperature over the year 1997 plus a number that is configurable from the recipe.

The recipe examples/recipe\_decadal.yml showcases how the timerange tag can be used to load datasets belonging to the DCPP activity. Produces timeseries plots comparing the global mean temperature of a DCPP dataset with an observational dataset.

### 18.4.2 Available recipes and diagnostics

#### Recipes are stored in esmvaltool/recipes/:

- examples/recipe\_python.yml
- examples/recipe\_easy\_ipcc.yml
- examples/recipe\_extract\_shape.yml
- examples/recipe\_julia.yml
- examples/recipe\_decadal.yml

#### Diagnostics are stored in esmvaltool/diag\_scripts/:

- examples/diagnostic.py: visualize results and store provenance information
- examples/make\_plot.py: Create a timeseries plot with likely ranges
- examples/diagnostic.jl: visualize results and store provenance information
- examples/decadal\_example.py: visualize results and store provenance information

### 18.4.3 User settings in recipe

1. Script examples/diagnostic.py

Required settings for script

- quickplot: plot\_type: which of the iris.quickplot functions to use. Arguments that are accepted by these functions can also be specified here, e.g. cmap. Preprocessors need to be configured such that the resulting data matches the plot type, e.g. a timeseries or a map.
- 2. Script examples/diagnostic.jl

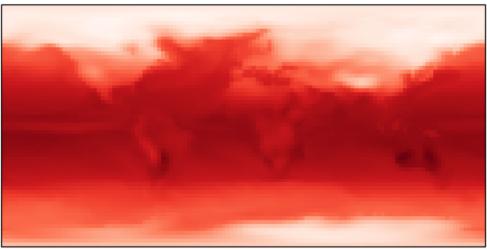
Required settings for script

• parameter1: example parameter, this number will be added to the mean (over time) value of the input data.

### 18.4.4 Variables

- tas (atmos, monthly, longitude, latitude, time)
- tos (ocean, monthly, longitude, latitude, time)

## 18.4.5 Example plots



## Air temperature

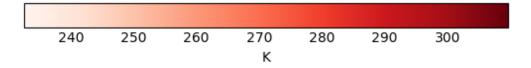


Fig. 41: Air temperature in January 2000 (BCC-ESM1 CMIP6).

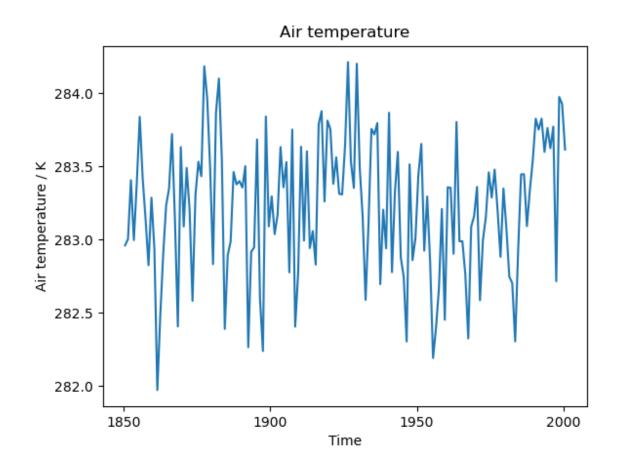


Fig. 42: Amsterdam air temperature (multimodel mean of CMIP5 CanESM2 and CMIP6 BCC-ESM1).

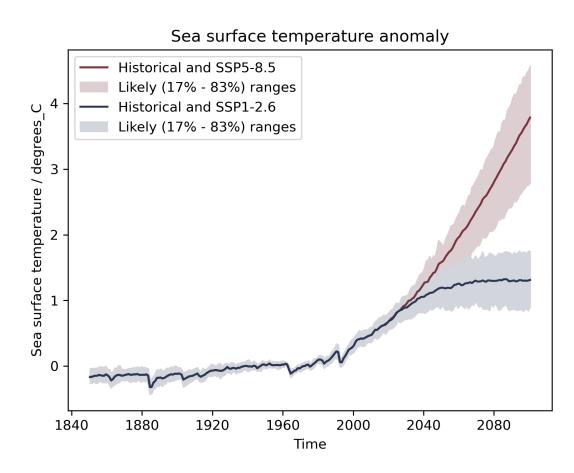


Fig. 43: Mean sea surface temperature anomaly (part of figure 9.3a from IPCC AR6).

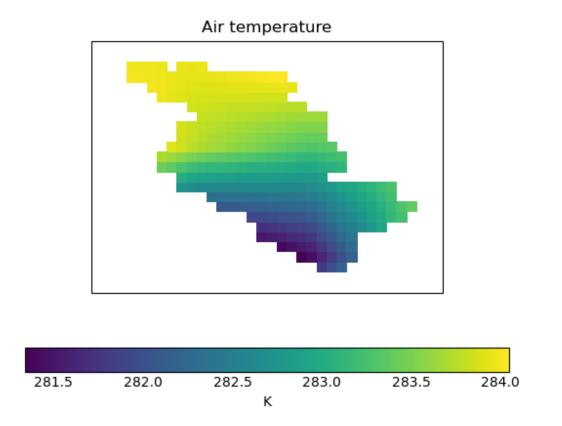


Fig. 44: Mean air temperature over the Elbe catchment during 2000-2002 according to CMIP5 CanESM2.

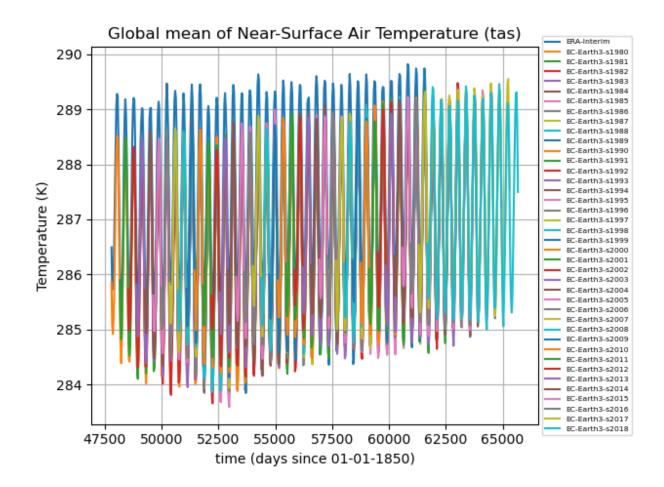


Fig. 45: Global mean temperature of CMIP6 dcppA-hindcast EC-Earth3 and OBS ERA-Interim.

### CHAPTER

## NINETEEN

## LAND

## 19.1 Landcover - Albedo

### 19.1.1 Overview

The diagnostic determines the coefficients of multiple linear regressions fitted between the albedo values and the tree, shrub, short vegetation (crops and grasses) fractions of each grid cell within spatially moving windows encompassing 5x5 model grid cells. Solving these regressions provides the albedo values for trees, shrubs and short vegetation (crops and grasses) from which the albedo changes associated with transitions between these three landcover types are derived. The diagnostic distinguishes between snow-free and snow-covered grid cells.

### 19.1.2 Available recipes and diagnostics

Recipes are stored in recipes/

recipe\_albedolandcover.yml

Diagnostics are stored in diag\_scripts/landcover/

· albedolandcover.py

### 19.1.3 User settings

Several parameters can be set in the recipe

### 19.1.4 Variables

- rsus (atmos, monthly mean, time latitude longitude)
- rsds (atmos, monthly mean, time latitude longitude)
- snc (landice, monthly mean, time latitude longitude)
- grassFrac (land, monthly mean, time latitude longitude)
- treeFrac (land, monthly mean, time latitude longitude)
- shrubFrac (land, monthly mean, time latitude longitude)
- cropFrac (land, monthly mean, time latitude longitude)
- pastureFrac (land, monthly mean, time latitude longitude)

## 19.1.5 Observations and reformat scripts

#### A reformatting script for observational data is available here:

• esmvaltool/cmorizers/data/formatters/datasets/duveiller2018.py

### 19.1.6 References

- Duveiller, G., Hooker, J. and Cescatti, A., 2018a. A dataset mapping the potential biophysical effects of vegetation cover change. Scientific Data, 5: 180014.
- Duveiller, G., Hooker, J. and Cescatti, A., 2018b. The mark of vegetation change on Earth's surface energy balance. Nature communications, 9(1): 679.

### 19.1.7 Example plots

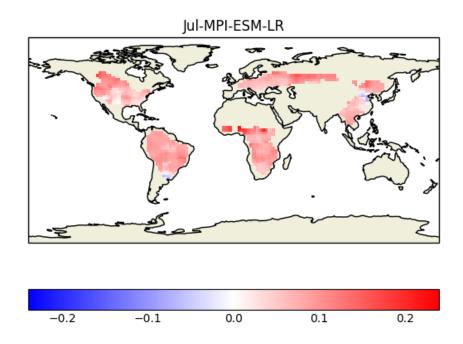


Fig. 1: Example of albedo change from tree to crop and grass for the CMIP5 model MPI-ESM-LR derived for the month of July and averaged over the years 2000 to 2004.

## 19.2 Turnover time of carbon over land ecosystems

### 19.2.1 Overview

This recipe evaluates the turnover time of carbon over land ecosystems (tau\_ctotal) based on the analysis of Carvalhais et al. (2014). In summary, it provides an overview on:

- Comparisons of global distributions of tau\_ctotal from all models against observation and other models
- Variation of tau\_ctotal across latitude (zonal distributions)
- Variation of association of tau\_ctotal and climate across latitude (zonal correlations)
- metrics of global tau\_ctotal and correlations

### 19.2.2 Calculation of turnover time

First, the total carbon content of land ecosystems is calculated as,

$$ctotal = cSoil + cVeg$$

where cSoil and cVeg are the carbon contents in soil and vegetation. Note that this is not fully consistent with `Carvalhais et al. (2014)`\_, in which `ctotal` includes all carbon storages that respire to the atmosphere. Due to inconsistency across models, it resulted in having different carbon storage components in calculation of ctotal for different models.

The turnover time of carbon is then calculated as,

$$\tau_{ctotal} = \frac{ctotal}{gpp}$$

where *ctotal* and *gpp* are temporal means of total carbon content and gross primary productivity, respectively. **The equation is valid for steady state, and is only applicable when both ctotal and gpp are long-term averages.** Therefore, the recipe should always include the mean operator of climate\_statistics in preprocessor.

### 19.2.3 Available recipes and diagnostics

Recipes are stored in recipes/

• recipe\_carvalhais14nat.yml

Diagnostics are stored in diag\_scripts/

- land\_carbon\_cycle/diag\_global\_turnover.py
- land\_carbon\_cycle/diag\_zonal\_turnover.py
- land\_carbon\_cycle/diag\_zonal\_correlation.py

## 19.2.4 User settings in recipe

#### **Observation-related details**

The settings needed for loading the observational dataset in all diagnostics are provided in the recipe through *obs\_info* within *obs\_details* section.

- obs\_data\_subdir: subdirectory of auxiliary\_data\_dir (set in config-user file) where observation data are stored {e.g., data\_ESMValTool\_Carvalhais2014}.
- source\_label: source data label {'Carvalhais2014'}.
- variant\_label: variant of the observation {'BE'} for best estimate.
- grid\_label: label denoting the spatial grid specification {'gn'}.
- frequency: temporal frequency of the observation data { 'fx' }

The observation data file used in the recipe should be changed through the fields above, as these are used to generate observation file name and locations. For details, see *Observations* section.

#### Preprocessor

- climate\_statistics: {mean} calculate the mean over full time period.
- regrid: {nearest} nearest neighbor regridding to the selected observation resolution.
- mask\_landsea: {sea} mask out all the data points from sea.
- multi\_model\_statistics: {median} calculate and include the multimodel median.

#### Script land\_carbon\_cycle/diag\_global\_turnover.py

- Required settings:
  - obs\_variable: {str} list of the variable(s) to be read from the observation files
- Optional settings:
  - ax\_fs: {float, 7.1} fontsize in the figure.
  - fill\_value: {float, nan} fill value to be used in analysis and plotting.
  - x0: {float, 0.02} X coordinate of the left edge of the figure.
  - y0: {float, 1.0} Y coordinate of the upper edge of the figure.
  - wp: {float, 1 / number of models} width of each map.
  - hp: {float, = wp} height of each map.
  - xsp: {float, 0} spacing betweeen maps in X direction.
  - ysp: {float, -0.03} spacing between maps in Y -direction. Negative to reduce the spacing below default.
  - aspect\_map: {float, 0.5} aspect of the maps.
  - xsp\_sca: {float, wp / 1.5} spacing between the scatter plots in X direction.
  - ysp\_sca: {float, hp / 1.5} spacing between the scatter plots in Y direction.
  - hcolo: {float, 0.0123} height (thickness for horizontal orientation) of the colorbar.
  - wcolo: {float, 0.25} width (length) of the colorbar.

- cb\_off\_y: {float, 0.06158} distance of colorbar from top of the maps.
- x\_colo\_d: {float, 0.02} X coordinate of the colorbar for maps along the diagonal (left).
- x\_colo\_r: {float, 0.76} Y coordinate of the colorbar for ratio maps above the diagonal (right).
- y\_colo\_single: {float, 0.1086} Y-coordinate of the colorbar in the maps per model (separate figures).
- correlation\_method: {str, spearman | pearson} correlation method to be used while calculating the correlation displayed in the scatter plots.
- tx\_y\_corr: {float, 1.075} Y coordinate of the inset text of correlation.
- valrange\_sc: {tuple, (2, 256)} range of turnover times in X and Y axes of scatter plots.
- obs\_global: {float, 23} global turnover time, provided as additional info for map of the observation. For models, they are calculated within the diagnostic.
- gpp\_threshold: {float, 0.01} The threshold of gpp in  $kg m^{-2} yr^{-1}$  below which the grid cells are masked.

#### Script land\_carbon\_cycle/diag\_zonal\_turnover.py

- Required settings:
  - obs\_variable: {str} list of the variable(s) to be read from the observation files
- Optional settings:
  - ax\_fs: {float, 7.1} fontsize in the figure.
  - fill\_value: {float, nan} fill value to be used in analysis and plotting.
  - valrange\_x: {tuple, (2, 1000)} range of turnover values in the X axis.
  - valrange\_y: {tuple, (-70, 90)} range of latitudes in the Y axis.
  - bandsize: {float, 9.5} size of the latitudinal rolling window in degrees. One latitude row if set to None.
  - gpp\_threshold: {float, 0.01} The threshold of gpp in  $kg m^{-2} yr^{-1}$  below which the grid cells are masked.

#### Script land\_carbon\_cycle/diag\_zonal\_correlation.py

- Required settings:
  - obs\_variable: {str} list of the variable(s) to be read from the observation files
- Optional settings:
  - ax\_fs: {float, 7.1} fontsize in the figure.
  - fill\_value: {float, nan} fill value to be used in analysis and plotting.
  - correlation\_method: {str, pearson | spearman} correlation method to be used while calculating the zonal correlation.
  - min\_points\_frac: {``float, 0.125} minimum fraction of valid points within the latitudinal band for calculation of correlation.
  - valrange\_x: {tuple, (-1, 1)} range of correlation values in the X axis.
  - valrange\_y: {tuple, (-70, 90)} range of latitudes in the Y axis.

- bandsize: {float, 9.5} size of the latitudinal rolling window in degrees. One latitude row if set to None.
- gpp\_threshold: {float, 0.01} The threshold of gpp in  $kg m^{-2} yr^{-1}$  below which the grid cells are masked.

## **19.2.5 Required Variables**

- *tas* (atmos, monthly, longitude, latitude, time)
- pr (atmos, monthly, longitude, latitude, time)
- *gpp* (land, monthly, longitude, latitude, time)
- *cVeg* (land, monthly, longitude, latitude, time)
- *cSoil* (land, monthly, longitude, latitude, time)

### 19.2.6 Observations

The observations needed in the diagnostics are publicly available for download from the Data Portal of the Max Planck Institute for Biogeochemistry after registration.

Due to inherent dependence of the diagnostic on uncertainty estimates in observation, the data needed for each diagnostic script are processed at different spatial resolutions (as in Carvalhais et al., 2014), and provided in 11 different resolutions (see Table 1). Note that the uncertainties were estimated at the resolution of the selected models, and, thus, only the pre-processed observed data can be used with the recipe. It is not possible to use regriding functionalities of ESMValTool to regrid the observational data to other spatial resolutions, as the uncertainty estimates cannot be regridded.

Reference	target_grid	grid_label*
Observation	0.5x0.5	gn
NorESM1-M	2.5x1.875	gr
bcc-csm1-1	2.812x2.813	gr1
CCSM4	1.25x0.937	gr2
CanESM2	2.812x2.813	gr3
GFDL-ESM2G	2.5x2.0	gr4
HadGEM2-ES	1.875x1.241	gr5
inmcm4	2.0x1.5	gr6
IPSL-CM5A-MR	2.5x1.259	gr7
MIROC-ESM	2.812x2.813	gr8
MPI-ESM-LR	1.875x1.875	gr9

Table 1. A summary of the observation datasets at different resolutions.

\* The grid\_label is suffixed with z for data in zonal/latitude coordinates: the zonal turnover and zonal correlation.

To change the spatial resolution of the evaluation, change {grid\_label} in obs\_details and the corresponding {target\_grid} in regrid preprocessor of the recipe.

At each spatial resolution, four data files are provided:

- tau\_ctotal\_fx\_Carvalhais2014\_BE\_gn.nc global data of tau\_ctotal
- tau\_ctotal\_fx\_Carvalhais2014\_BE\_gnz.nc zonal data of tau\_ctotal

- r\_tau\_ctotal\_tas\_fx\_Carvalhais2014\_BE\_gnz.nc zonal correlation of tau\_ctotal and tas, controlled for pr
- r\_tau\_ctotal\_pr\_fx\_Carvalhais2014\_BE\_gnz.nc zonal correlation of tau\_ctotal and pr, controlled for tas.

The data is produced in obs4MIPs standards, and provided in netCDF4 format. The filenames use the convention:

{variable}\_{frequency}\_{source\_label}\_{variant\_label}\_{grid\_label}.nc

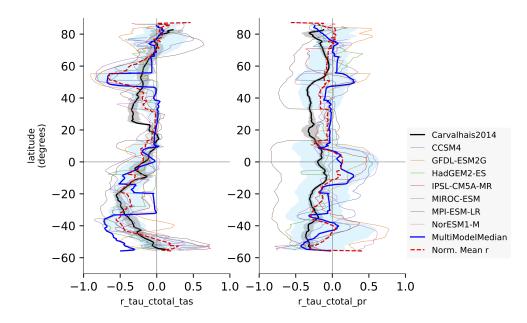
- {variable}: variable name, set in every diagnostic script as obs\_variable
- {frequency}: temporal frequency of data, set from obs\_details
- {source\_label}: observational source, set from obs\_details
- {variant\_label}: observation variant, set from obs\_details
- {grid\_label}: temporal frequency of data, set from obs\_details

Refer to the Obs4MIPs Data Specifications for details of the definitions above.

All data variables have additional variables ({variable}\_5 and {variable}\_95) in the same file. These variables are necessary for a successful execution of the diagnostics.

### 19.2.7 References

• Carvalhais, N., et al. (2014), Global covariation of carbon turnover times with climate in terrestrial ecosystems, Nature, 514(7521), 213-217, doi: 10.1038/nature13731.



### 19.2.8 Example plots

Fig. 2: Comparison of latitudinal (zonal) variations of pearson correlation between turnover time and climate: turnover time and precipitation, controlled for temperature (left) and vice-versa (right). Reproduces figures 2c and 2d in Carvalhais et al. (2014).

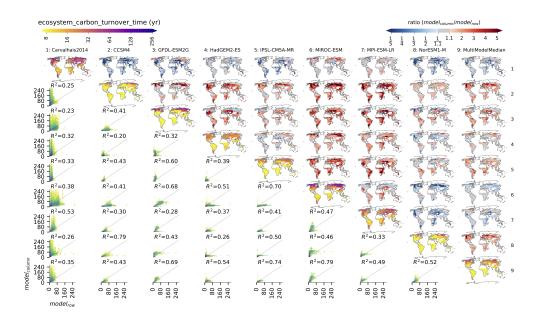


Fig. 3: Comparison of observation-based and modelled ecosystem carbon turnover time. Along the diagnonal, tau\_ctotal are plotted, above the bias, and below density plots. The inset text in density plots indicate the correlation.

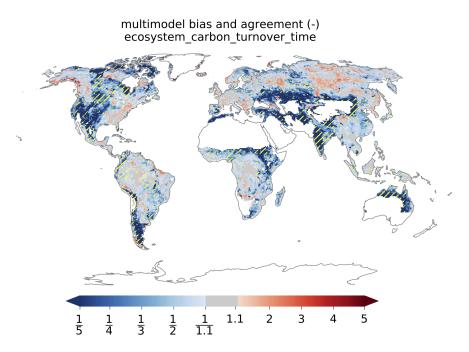


Fig. 4: Global distributions of multimodel bias and model agreement. Multimodel bias is calculated as the ratio of multimodel median turnover time and that from observation. Stippling indicates the regions where only less than one quarter of the models fall within the range of observational uncertainties ( $5^{th}$  and  $95^{th}$  percentiles). Reproduces figure 3 in Carvalhais et al. (2014).

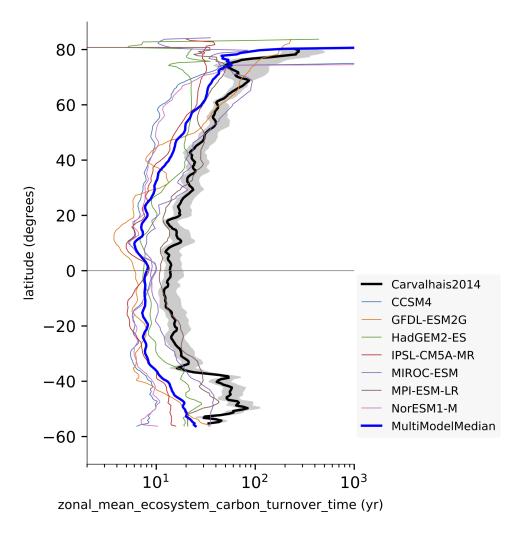


Fig. 5: Comparison of latitudinal (zonal) variations of observation-based and modelled ecosystem carbon turnover time. The zonal turnover time is calculated as the ratio of zonal *ctotal* and *gpp*. Reproduces figures 2a and 2b in Carvalhais et al. (2014).

# **19.3 Hydrological models - data pre-processing**

### 19.3.1 Overview

We provide a collection of scripts that pre-processes environmental data for use in several hydrological models:

#### PCR-GLOBWB

PCR-GLOBWB (PCRaster Global Water Balance) is a large-scale hydrological model intended for global to regional studies and developed at the Department of Physical Geography, Utrecht University (Netherlands). The recipe preprocesses ERA-Interim reanalyses data for use in the PCR-GLOBWB.

#### MARRMoT

MARRMoT (Modular Assessment of Rainfall-Runoff Models Toolbox) is a rainfall-runoff model comparison framework that allows objective comparison between different conceptual hydrological model structures https://github.com/ wknoben/MARRMoT. The recipe pre-processes ERA-Interim and ERA5 reanalyses data for use in the MARRMoT.

MARRMoT requires potential evapotranspiration (evspsblpot). The variable evspsblpot is not available in ERA-Interim. Thus, we use the debruin function (De Bruin et al. 2016) to obtain evspsblpot using both ERA-Interim and ERA5. This function needs the variables tas, psl, rsds, and rsdt as input.

#### wflow\_sbm and wflow\_topoflex

Forcing data for the wflow\_sbm and wflow\_topoflex hydrological models can be prepared using recipe\_wflow.yml. If PET is not available from the source data (e.g. ERA-Interim), then it can be derived from psl, rsds and rsdt using De Bruin's 2016 formula (De Bruin et al. 2016). For daily ERA5 data, the time points of these variables are shifted 30 minutes with respect to one another. This is because in ERA5, accumulated variables are recorded over the past hour, and in the process of cmorization, we shift the time coordinates to the middle of the interval over which is accumulated. However, computing daily statistics then averages the times, which results in 12:00 UTC for accumulated variables and 11:30 UTC for instantaneous variables. Therefore, in this diagnostic, the time coordinates of the daily instantaneous variables are shifted 30 minutes forward in time.

#### LISFLOOD

LISFLOOD is a spatially distributed water resources model, developed by the Joint Research Centre (JRC) of the European Commission since 1997. We provide a recipe to produce meteorological forcing data for the Python 3 version of LISFLOOD.

LISFLOOD has a separate preprocessor LISVAP that derives some additional variables. We don't replace LISVAP. Rather, we provide input files that can readily be passed to LISVAP and then to LISFLOOD.

#### HYPE

The hydrological catchment model HYPE simulates water flow and substances on their way from precipitation through soil, river and lakes to the river outlet. HYPE is developed at the Swedish Meteorological and Hydrological Institute. The recipe pre-processes ERA-Interim and ERA5 data for use in HYPE.

#### GlobWat

GlobWat is a soil water balance model that has been provided by the Food and Agriculture Organization (FAO) to assess water use in irrigated agriculture (http://www.fao.org/nr/water/aquamaps). The recipe pre-processes ERA-Interim and ERA5 reanalyses data for use in the GlobWat model. GlobWat requires potential evapotranspiration (evspsblpot) as input. The variable evspsblpot is not available in ERA-Interim. Thus, we use debruin function (De Bruin et al. 2016) or the langbein method (Langbein et al. 1949) to obtain evspsblpot using both ERA-Interim and ERA5. The Langbein function needs a variable tas and the debruin function besides that needs the variables psl, rsds, and rsdt as input. In order to calculate monthly/daily pet with Langbein method we assumed that tas is constant over time and the average value is equal to the annual average.

### 19.3.2 Available recipes and diagnostics

Recipes are stored in esmvaltool/recipes/hydrology

- recipe\_pcrglobwb.yml
- recipe\_marrmot.yml
- recipe\_wflow.yml
- recipe\_lisflood.yml
- recipe\_hype.yml
- · recipe\_globwat.yml

Diagnostics are stored in esmvaltool/diag\_scripts/hydrology

- pcrglobwb.py
- marrmot.py
- wflow.py
- lisflood.py
- hype.py
- globwat.py

#### 19.3.3 User settings in recipe

All hydrological recipes require a shapefile as an input to produce forcing data. This shapefile determines the shape of the basin for which the data will be cut out and processed. All recipes are tested with the shapefiles that are used for the eWaterCycle project. In principle any shapefile can be used, for example, the freely available basin shapefiles from the HydroSHEDS project.

1. recipe\_pcrglobwb.yml

Required preprocessor settings:

• start\_year: 1979

- end\_year: 1979
- 2. recipe\_marrmot.yml

There is one diagnostic diagnostic\_daily for using daily data.

Required preprocessor settings:

The settings below should not be changed.

extract\_shape:

- shapefile: Meuse.shp (MARRMoT is a hydrological Lumped model that needs catchmentaggregated forcing data. The catchment is provided as a shapefile, the path can be relative to auxiliary\_data\_dir as defined in config-user.yml.).
- method: contains
- crop: true

Required diagnostic script settings:

- basin: Name of the catchment
- 3. recipe\_wflow.yml

Optional preprocessor settings:

• extract\_region: the region specified here should match the catchment

Required diagnostic script settings:

- basin: name of the catchment
- dem\_file: netcdf file containing a digital elevation model with elevation in meters and coordinates latitude and longitude. A wflow example dataset is available at: https://github.com/openstreams/wflow/ tree/master/examples/wflow\_rhine\_sbm The example dem\_file can be obtained from https://github.com/ openstreams/wflow/blob/master/examples/wflow\_rhine\_sbm/staticmaps/wflow\_dem.map
- regrid: the regridding scheme for regridding to the digital elevation model. Choose area\_weighted (slow) or linear.
- 4. recipe\_lisflood.yml

Required preprocessor settings:

- extract\_region: A region bounding box slightly larger than the shapefile. This is run prior to regridding, to save memory.
- extract\_shape:\*
  - shapefile: A shapefile that specifies the extents of the catchment.

These settings should not be changed

- method: contains
- crop: true
- regrid:\*
  - target\_grid: Grid of LISFLOOD input files

These settings should not be changed

- lon\_offset: true
- lat\_offset: true

- scheme: linear

There is one diagnostic diagnostic\_daily for using daily data.

Required diagnostic script settings:

- catchment: Name of the catchment, used in output filenames
- 5. recipe\_hype.yml

Required preprocessor settings:

- start\_year: 1979
- end\_year: 1979
- shapefile: Meuse\_HYPE.shp (expects shapefile with subcatchments)

These settings should not be changed

- · method: contains
- · decomposed: true
- 6. recipe\_globwat.yml

Required preprocessor settings:

- start\_year: 2004
- end\_year: 2004
- target\_grid\_file: grid of globwat input files. A target file has been generated from one of the GlobWat models sample files (prc01wb.asc) for regridding ERA5 and ERA-Interim datasets. The ASCII file can be found at: https://storage.googleapis.com/fao-maps-catalog-data/geonetwork/aquamaps/GlobWat-InputP1\_prec. zip. You can use the GDAL translator to convert the file from ASCII format to NetCDF format by entering the following command into the terminal: gdal\_translate -of netCDF prc01wb.asc globwat\_target\_grid.nc

Optional preprocessor settings:

- area\_selection: A region bounding box to extract the data for a specific region. The area selection preprocessor can be used by users to process the data for their desired region. The data will be processed at the global scale if the preprocessor in the recipe is commented.
- regrid\_scheme: The area-weighted regridding scheme is used as a default regridding scheme to ensure that the total volume of water is consistent before and after regridding.
- langbein\_pet: Can be set to True to use langbein function for calculating evspsblpot (default is de bruin method)

#### **19.3.4 Variables**

- 1. recipe\_pcrglobwb.yml
  - tas (atmos, daily, longitude, latitude, time)
  - pr (atmos, daily, longitude, latitude, time)
- 2. recipe\_marrmot.yml
  - pr (atmos, daily or hourly mean, longitude, latitude, time)
  - psl (atmos, daily or hourly mean, longitude, latitude, time)
  - rsds (atmos, daily or hourly mean, longitude, latitude, time)
  - rsdt (atmos, daily or hourly mean, longitude, latitude, time)

- tas (atmos, daily or hourly mean, longitude, latitude, time)
- 3. recipe\_wflow.yml
  - orog (fx, longitude, latitude)
  - pr (atmos, daily or hourly mean, longitude, latitude, time)
  - tas (atmos, daily or hourly mean, longitude, latitude, time)

Either potential evapotranspiration can be provided:

• evspsblpot(atmos, daily or hourly mean, longitude, latitude, time)

or it can be derived from tas, psl, rsds, and rsdt using the De Bruin formula, in that case the following variables need to be provided:

- psl (atmos, daily or hourly mean, longitude, latitude, time)
- rsds (atmos, daily or hourly mean, longitude, latitude, time)
- rsdt (atmos, daily or hourly mean, longitude, latitude, time)
- 4. recipe\_lisflood.yml
  - pr (atmos, daily, longitude, latitude, time)
  - tas (atmos, daily, longitude, latitude, time)
  - tasmax (atmos, daily, longitude, latitude, time)
  - tasmin (atmos, daily, longitude, latitude, time)
  - tdps (atmos, daily, longitude, latitude, time)
  - uas (atmos, daily, longitude, latitude, time)
  - vas (atmos, daily, longitude, latitude, time)
  - rsds (atmos, daily, longitude, latitude, time)
- 5. recipe\_hype.yml
  - tas (atmos, daily or hourly, longitude, latitude, time)
  - tasmin (atmos, daily or hourly, longitude, latitude, time)
  - tasmax (atmos, daily or hourly, longitude, latitude, time)
  - pr (atmos, daily or hourly, longitude, latitude, time)
- 6. recipe\_globwat.yml
  - pr (atmos, daily or monthly, longitude, latitude, time)
  - tas (atmos, daily or monthly, longitude, latitude, time)
  - psl (atmos, daily or monthly, longitude, latitude, time)
  - rsds (atmos, daily or monthly, longitude, latitude, time)
  - rsdt (atmos, daily or monthly, longitude, latitude, time)

### 19.3.5 Observations and reformat scripts

Note: download instructions can be obtained with `esmvaltool data info DATASET` or in headers of cmorization scripts.

- ERA-Interim (esmvaltool/cmorizers/data/formatters/datasets/era\_interim.py)
- ERA5 (esmvaltool/diag\_scripts/cmorizers/era5.py)

### 19.3.6 Output

- 1. recipe\_pcrglobwb.yml
- 2. recipe\_marrmot.yml

The forcing data, the start and end times of the forcing data, the latitude and longitude of the catchment are saved in a .mat file as a data structure readable by MATLAB or Octave.

3. recipe\_wflow.yml

The forcing data, stored in a single NetCDF file.

4. recipe\_lisflood.yml

The forcing data, stored in separate files per variable.

5. recipe\_globwat.yml

The forcing data, stored in separate files per timestep and variable.

### 19.3.7 References

- Sutanudjaja, E. H., van Beek, R., Wanders, N., Wada, Y., Bosmans, J. H. C., Drost, N., van der Ent, R. J., de Graaf, I. E. M., Hoch, J. M., de Jong, K., Karssenberg, D., López López, P., Peßenteiner, S., Schmitz, O., Straatsma, M. W., Vannametee, E., Wisser, D., and Bierkens, M. F. P.: PCR-GLOBWB 2: a 5arcmin global hydrological and water resources model, Geosci. Model Dev., 11, 2429-2453, https://doi.org/10.5194/gmd-11-2429-2018, 2018.
- De Bruin, H. A. R., Trigo, I. F., Bosveld, F. C., Meirink, J. F.: A Thermodynamically Based Model for Actual Evapotranspiration of an Extensive Grass Field Close to FAO Reference, Suitable for Remote Sensing Application, American Meteorological Society, 17, 1373-1382, DOI: 10.1175/JHM-D-15-0006.1, 2016.
- Arheimer, B., Lindström, G., Pers, C., Rosberg, J. och J. Strömqvist, 2008. Development and test of a new Swedish water quality model for small-scale and large-scale applications. XXV Nordic Hydrological Conference, Reykjavik, August 11-13, 2008. NHP Report No. 50, pp. 483-492.
- Lindström, G., Pers, C.P., Rosberg, R., Strömqvist, J., Arheimer, B. 2010. Development and test of the HYPE (Hydrological Predictions for the Environment) model – A water quality model for different spatial scales. Hydrology Research 41.3-4:295-319.
- van der Knijff, J. M., Younis, J. and de Roo, A. P. J.: LISFLOOD: A GIS-based distributed model for river basin scale water balance and flood simulation, Int. J. Geogr. Inf. Sci., 24(2), 189–212, 2010.
- Hoogeveen, J., Faurès, J. M., Peiser, L., Burke, J., de Giesen, N. V.: GlobWat–a global water balance model to assess water use in irrigated agriculture, Hydrology & Earth System Sciences Discussions, 2015 Jan 1;12(1), Doi:10.5194/hess-19-3829-2015.
- Langbein, W.B., 1949. Annual runoff in the United States. US Geol. Surv.(https://pubs.usgs.gov/circ/1949/ 0052/report.pdf)

# 19.4 Hydro forcing comparison

### 19.4.1 Overview

This recipe can be used to assess the agreement between forcing datasets (i.e. MSWEP, ERA5, ERA-Interim) for a defined catchment. The recipe can be used to:

- 1. Plot a timeseries of the raw daily data
- 2. Plot monthly aggregrated data over a defined period
- 3. Plot the monthly / daily climatology statistics over a defined period

### 19.4.2 Available recipes and diagnostics

Recipes are stored in esmvaltool/recipes/hydrology

recipe\_hydro\_forcing.yml

Diagnostics are stored in esmvaltool/diag\_scripts/hydrology/

• hydro\_forcing.py: Compares and plots precipitation for MSWEP / ERA5 / ERA-5 interim datasets

## 19.4.3 User settings in recipe

All hydrological recipes require a shapefile as an input to select forcing data. This shapefile determines the shape of the basin for which the data will be cut out and processed. All recipes are tested with the shapefiles from HydroSHEDS that are used for the eWaterCycle project. In principle any shapefile can be used, for example, the freely available basin shapefiles from the HydroSHEDS project.

1. recipe hydrology/hydro\_forcing.yml

Optional preprocessor settings:

• extract\_shape: The region specified here should match the catchment

Required settings for script:

- plot\_type: Define which plot function to run. Choices:
  - timeseries: Plot a timeseries for the variable data over the defined period
  - climatology: Plot the climate statistics over the defined period

Required settings for ``timeseries `` plots:

• time\_period: Defines the period of the output for the correct captions/labels. This value should match the period used for the preprocessor. Choices: day, month.

## 19.4.4 Variables

• pr (atmos, daily or monthly, longitude, latitude, time)

## 19.4.5 Observations

All data can be used directly without any preprocessing.

- ERA-Interim
- ERA5
- MSWEP

## 19.4.6 Example plots

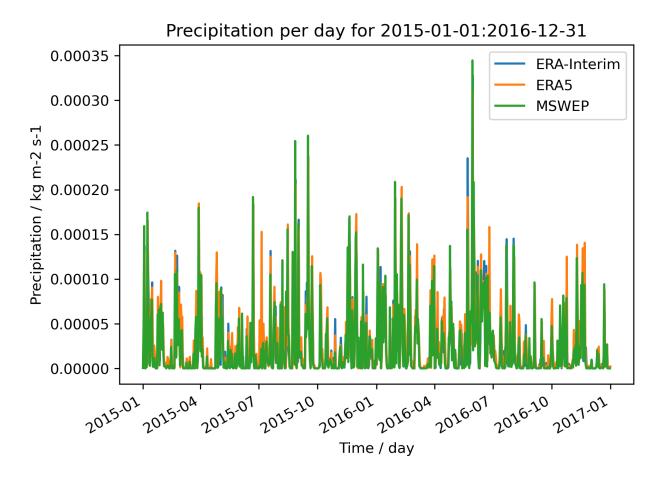


Fig. 6: Precipitation per day for 2015-01-01:2016-12-31.

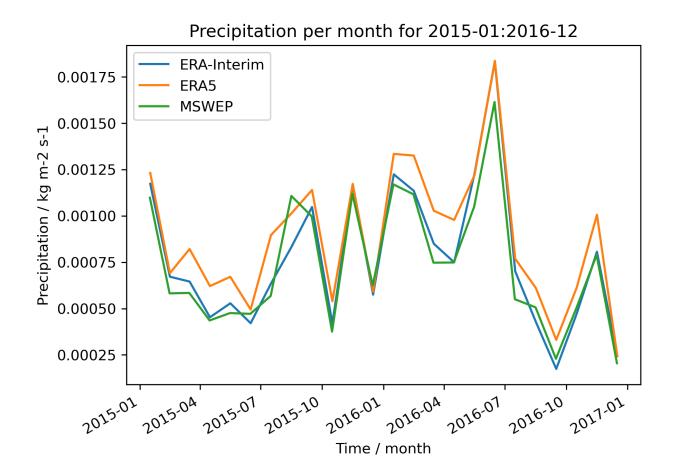


Fig. 7: Precipitation per month for 2015-01:2016-12.

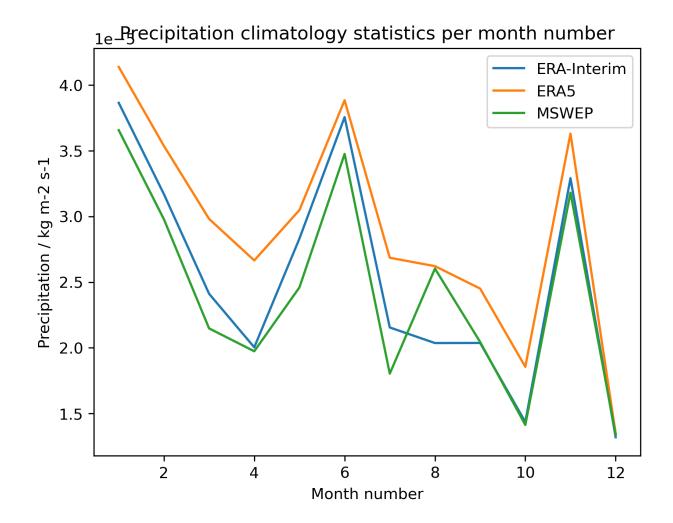


Fig. 8: Precipitation climatology statistics per month number.

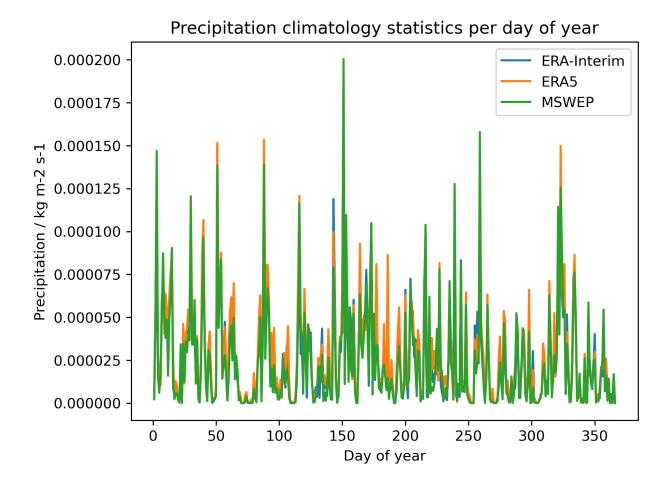


Fig. 9: Precipitation climatology statistics per day of year.

# **19.5 Landcover diagnostics**

### 19.5.1 Overview

The diagnostic computes the accumulated and fractional extent of major land cover classes, namely bare soil, crops, grasses, shrubs and trees. The numbers are compiled for the whole land surface as well as separated into Tropics, northern Extratropics and southern Extratropics. The cover fractions are compared to ESA-CCI land cover data.

### 19.5.2 Available recipes and diagnostics

Recipes are stored in recipes/

• recipe\_landcover.yml

Diagnostics are stored in diag\_scripts/landcover/

• landcover.py: bar plots showing the accumulated area and mean fractional coverage for five land cover classes for all experiments as well as their bias compared to observations.

## 19.5.3 User settings

script landcover.py

Required settings for script

• reference\_dataset: land cover extent dataset for comparison. The script was developed using ESACCI-LANDCOVER observations.

Optional settings for script

- comparison: [variable, model] Choose whether one plot per land cover class is generated comparing the different experiments (default) or one plot per model comparing the different land cover classes.
- colorscheme: Plotstyle used for the bar plots. A list of available style is found at https://matplotlib. org/gallery/style\_sheets/style\_sheets\_reference.html. Seaborn is used as default.

### 19.5.4 Variables

- baresoilFrac (land, monthly mean, time latitude longitude)
- grassFrac (land, monthly mean, time latitude longitude)
- treeFrac (land, monthly mean, time latitude longitude)
- shrubFrac (land, monthly mean, time latitude longitude)
- cropFrac (land, monthly mean, time latitude longitude)

## 19.5.5 Observations and reformat scripts

ESA-CCI land cover data (Defourny et al., 2015) needs to be downloaded manually by the user and converted to netCDF files containing the grid cell fractions for the five major land cover types. The data and a conversion tool are available at https://maps.elie.ucl.ac.be/CCI/viewer/ upon registration. After obtaining the data and the user tool, the remapping to 0.5 degree can be done with:

./bin/aggregate-map.sh -PgridName=GEOGRAPHIC\_LAT\_LON -PnumRows=360 -PoutputLCCSClasses=true -PnumMajorityClasses=0 ESACCI-LC-L4-LCCS-Map-300m-P1Y-2015-v2.0.7b.nc

Next, the data needs to be aggregated into the five major classes (PFT) similar to the study of Georgievski & Hagemann (2018) and converted from grid cell fraction into percentage.

PFT	ESA-CCI Landcover Classes
baresoil- Frac	Bare_Soil
cropFrac	Managed_Grass
grassFrac	Natural_Grass
shrubFrac	Shrub_Broadleaf_Deciduous + Shrub_Broadleaf_Evergreen + Shrub_Needleleaf_Evergreen
treeFrac	Tree_Broadleaf_Deciduous + Tree_Broadleaf_Evergreen + Tree_Needleleaf_Deciduous + Tree_Needleleaf_Evergreen

Finally, it might be necessary to adapt the grid structure to the experiments files, e.g converting the -180 -> 180 degree grid to 0 -> 360 degree and inverting the order of latitudes. Note, that all experiments will be regridded onto the grid of the land cover observations, thus it is recommended to convert to the coarses resolution which is sufficient for the planned study. For the script development, ESA-CCI data on 0.5 degree resolution was used with land cover data averaged over the 2008-2012 period.

### 19.5.6 References

- Defourny et al. (2015): ESA Land Cover Climate Change Initiative (ESA LC\_cci) data: ESACCI-LC-L4-LCCS-Map-300m-P5Y-[2000,2005,2010]-v1.6.1 via Centre for Environmental Data Analysis
- Georgievski, G. & Hagemann, S. Characterizing uncertainties in the ESA-CCI land cover map of the epoch 2010 and their impacts on MPI-ESM climate simulations, Theor Appl Climatol (2018). https://doi.org/10.1007/ s00704-018-2675-2

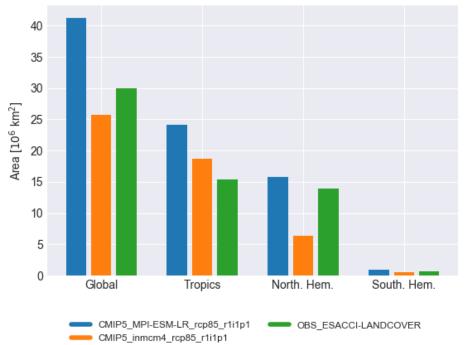
## 19.5.7 Example plots

# **19.6 Land and ocean components of the global carbon cycle**

### 19.6.1 Overview

This recipe reproduces most of the figures of Anav et al. (2013):

• Timeseries plot for different regions



Accumulated tree covered area

Fig. 10: Accumulated tree covered area for different regions and experiments.

- Seasonal cycle plot for different regions
- Errorbar plot for different regions showing mean and standard deviation
- · Scatterplot for different regions showing mean vs. interannual variability
- 3D-scatterplot for different regions showing mean vs. linear trend and the model variability index (MVI) as a third dimension (color coded)
- Scatterplot for different regions comparing two variable against each other (cSoil vs. cVeg)

In addition, performance metrics are calculated for all variables using the performance metric diagnostics (see details in *Performance metrics for essential climate parameters*).

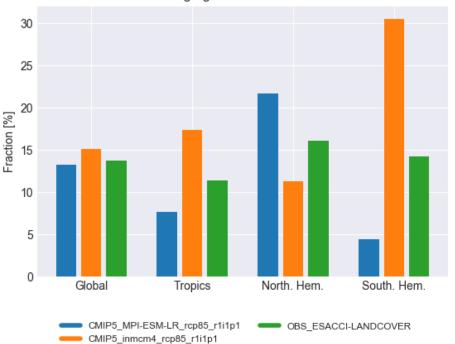
### 19.6.2 MVI calculation

The Model variability index (MVI) on a single grid point (calculated in carbon\_cycle/mvi.ncl is defined as

$$MVI = \left(\frac{s^M}{s^O} - \frac{s^O}{s^M}\right)^2$$

where  $s^M$  and  $s^O$  are the standard deviations of the annual time series on a single grid point of a climate model M and the reference observation O. In order to get a global or regional result, this index is simple averaged over the respective domain.

In its given form, this equation is prone to small standard deviations close to zero. For example, values of  $s^M = 10^{-5}\mu$  and  $s^O = 10^{-7}\mu$  (where  $\mu$  is the mean of  $s^O$  over all grid cells) results in a MVI of the order of  $10^4$  for this single grid



Average grass covered fraction

Fig. 11: Average grass cover fraction for different regions and experiments

cell even though the two standard deviations are close to zero and negligible compared to other grid cells. Due to the use of the arithmetic mean, a single high value is able to distort the overall MVI.

In the original publication, the maximum MVI is in the order of 10 (for the variable *gpp*). However, a naive application of the MVI definition yields values over  $10^9$  for some models. Unfortunately, Anav et al. (2013) do not provide an explanation on how to deal with this problem. Nevertheless, this script provides two configuration options to avoid high MVI values, but they are not related to the original paper or any other peer-revied study and should be used with great caution (see *User settings in recipe*).

## 19.6.3 Available recipes and diagnostics

Recipes are stored in recipes/

• recipe\_anav13jclim.yml

Diagnostics are stored in diag\_scripts/

- carbon\_cycle/main.ncl
- carbon\_cycle/mvi.ncl
- carbon\_cycle/two\_variables.ncl
- perfmetrics/main.ncl
- perfmetrics/collect.ncl

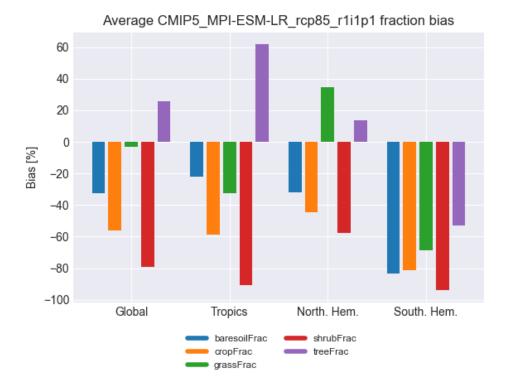


Fig. 12: Biases in five major land cover fractions for different regions and one experiment.

# 19.6.4 User settings in recipe

- 1. Preprocessor
  - mask\_fillvalues: Mask common missing values on different datasets.
  - mask\_landsea: Mask land/ocean.
  - regrid: Regridding.
  - weighting\_landsea\_fraction: Land/ocean fraction weighting.
- 2. Script carbon\_cycle/main.ncl
  - region, *str*: Region to be averaged.
  - legend\_outside, bool: Plot legend in a separate file (does not affect errorbar plot and evolution plot)
  - seasonal\_cycle\_plot, bool: Draw seasonal cycle plot.
  - errorbar\_plot, *bool*: Draw errorbar plot.
  - mean\_IAV\_plot, *bool*: Draw Mean (x-axis), IAV (y-axis) plot.
  - evolution\_plot, *bool*: Draw time evolution of a variable comparing a reference dataset to multi-dataset mean; requires ref\_dataset in recipe.
  - sort, *bool*, optional (default: False): Sort dataset in alphabetical order.
  - anav\_month, bool, optional (default: False): Conversion of y-axis to PgC/month instead of /year.

- evolution\_plot\_ref\_dataset, *str*, optional: Reference dataset for evolution\_plot. Required when evolution\_plot is True.
- evolution\_plot\_anomaly, str, optional (default: False): Plot anomalies in evolution plot.
- evolution\_plot\_ignore, *list*, optional: Datasets to ignore in evolution plot.
- evolution\_plot\_volcanoes, *bool*, optional (default: False): Turns on/off lines of volcano eruptions in evolution plot.
- evolution\_plot\_color, *int*, optional (default: 0): Hue of the contours in the evolution plot.
- ensemble\_name, string, optional: Name of ensemble for use in evolution plot legend
- 3. Script carbon\_cycle/mvi.ncl
  - region, *str*: Region to be averaged.
  - reference\_dataset, str: Reference dataset for the MVI calculation specified for each variable seperately.
  - mean\_time\_range, *list*, optional: Time period over which the mean is calculated (if not given, use whole time span).
  - trend\_time\_range, *list*, optional: Time period over which the trend is calculated (if not given, use whole time span).
  - mvi\_time\_range, *list*, optional: Time period over which the MVI is calculated (if not given, use whole time span).
  - stddev\_threshold, *float*, optional (default: 1e-2): Threshold to ignore low standard deviations (relative to the mean) in the MVI calculations. See also *MVI calculation*.
  - mask\_below, *float*, optional: Threshold to mask low absolute values (relative to the mean) in the input data (not used by default). See also *MVI calculation*.
- 4. Script carbon\_cycle/two\_variables.ncl
  - region, *str*: Region to be averaged.
- 5. Script perfmetrics/main.ncl

See Performance metrics for essential climate parameters.

6. Script perfmetrics/collect.ncl

See Performance metrics for essential climate parameters.

#### 19.6.5 Variables

- tas (atmos, monthly, longitude, latitude, time)
- pr (atmos, monthly, longitude, latitude, time)
- *nbp* (land, monthly, longitude, latitude, time)
- gpp (land, monthly, longitude, latitude, time)
- *lai* (land, monthly, longitude, latitude, time)
- *cveg* (land, monthly, longitude, latitude, time)
- csoil (land, monthly, longitude, latitude, time)
- tos (ocean, monthly, longitude, latitude, time)
- fgco2 (ocean, monthly, longitude, latitude, time)

### 19.6.6 Observations and reformat scripts

- CRU (tas, pr)
- JMA-TRANSCOM (*nbp*, *fgco2*)
- MTE (*gpp*)
- LAI3g (lai)
- NDP (cveg)
- HWSD (csoil)
- HadISST (tos)

## 19.6.7 References

• Anav, A. et al.: Evaluating the land and ocean components of the global carbon cycle in the CMIP5 Earth System Models, J. Climate, 26, 6901-6843, doi: 10.1175/JCLI-D-12-00417.1, 2013.

# 19.6.8 Example plots

# 19.7 Runoff, Precipitation, Evapotranspiration

## 19.7.1 Overview

This diagnostic calculates biases of long-term climatological annual means of total runoff R, precipitation P and evapotranspiration E for 12 large-scale catchments on different continents and climates. For total runoff, catchment averaged model values are compared to climatological GRDC station observations of river runoff (Duemenil Gates et al., 2000). Due to the incompleteness of these station data, a year-to-year correspondence of data cannot be achieved in a generalized way, so that only climatological data are considered, such it has been done in Hagemann, et al. (2013). For precipitation, catchment-averaged WFDEI precipitation data (Weedon et al., 2014) from 1979-2010 is used as reference. For evapotranspiration, observations are estimated using the difference of the above mentioned precipitation reference minus the climatological GRDC river runoff.

The catchments are Amazon, Congo, Danube, Ganges-Brahmaputra, Lena, Mackenzie, Mississippi, Murray, Niger, Nile, Parana and Yangtze-Kiang. Variable names are expected to follow CMOR standard, e.g. precipitation as pr, total runoff as mrro and evapotranspiration as evspsbl with all fluxes given in kg m-2 s-1. Evapotranspiration furthermore has to be defined positive upwards.

The diagnostic produces text files with absolute and relative bias to the observations, as well as the respective absolute values. Furthermore it creates a bar plot for relative and absolute bias, calculates and plots biases in runoff coefficient (R/P) and evapotranspiration coefficient (E/P) and saves everything as one pdf file per model or one png file per model and analysis.

The bias of the runoff coefficient is calculated via:  $C_R = \frac{R_{model}}{P_{model}} - \frac{R_{GRDC}}{P_{WFDEI}}$  and similar for the evapotranspiration coefficient. In a very first approximation, evapotranspiration and runoff are determined only by precipitation. In other words R = P - E. Hence, the runoff coefficient (and similar the evapotranspiration coefficient) tells you how important runoff (or evapotranspiration) is in this region. By plotting the bias of the runoff coefficient against the evapotranspiration coefficient we can immediately see whether there is a shift from runoff to evapotranspiration. On the other hand, by plotting the bias of the runoff coefficient against the relative bias of precipitation we can see whether an error in runoff is due to an error in precipitation.

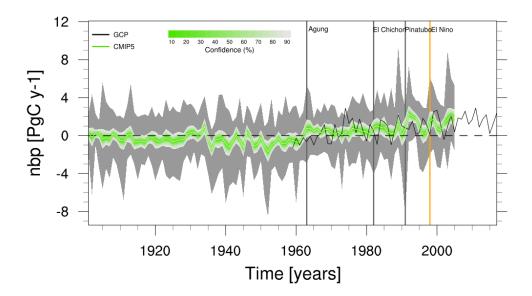


Fig. 13: Time series of global net biome productivity (NBP) over the period 1901-2005. Similar to Anav et al. (2013), Figure 5.

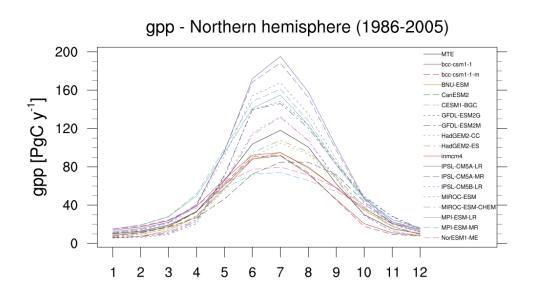


Fig. 14: Seasonal cycle plot for nothern hemisphere gross primary production (GPP) over the period 1986-2005. Similar to Anav et al. (2013), Figure 9.

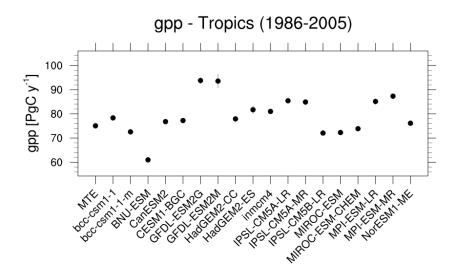


Fig. 15: Errorbar plot for tropical gross primary production (GPP) over the period 1986-2005.

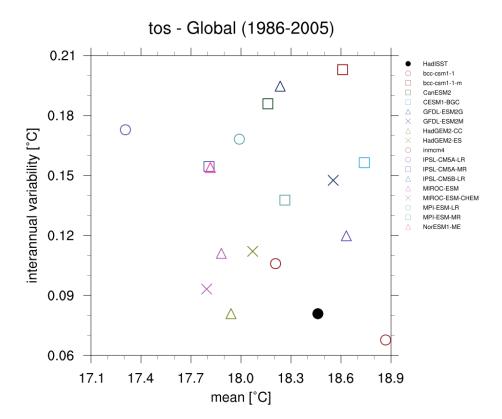


Fig. 16: Scatterplot for interannual variability and mean of global sea surface temperature (TOS) over the period 1986-2005.

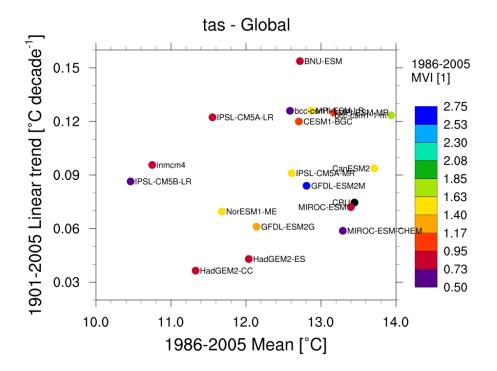


Fig. 17: Scatterplot for multiyear average of 2m surface temperature (TAS) in x axis, its linear trend in y axis, and MVI. Similar to Anav et al. (2013) Figure 1 (bottom).

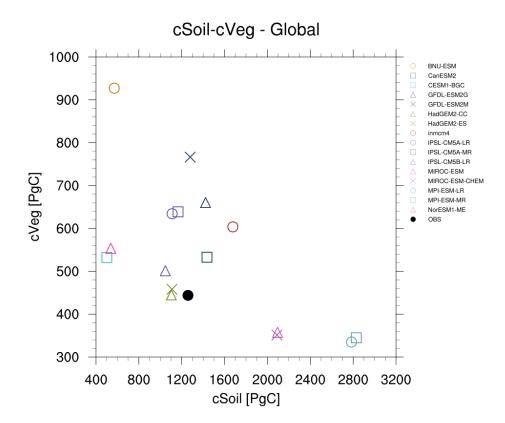


Fig. 18: Scatterplot for vegetation carbon content (cVeg) and soil carbon content (cSoil) over the period 1986-2005. Similar to Anav et al. (2013), Figure 12.

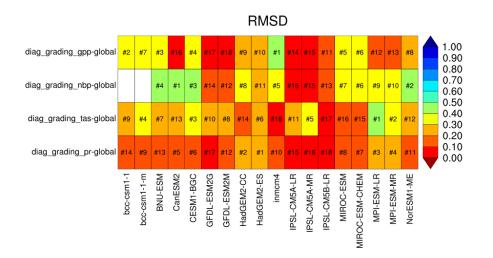


Fig. 19: Performance metrics plot for carbon-cycle-relevant diagnostics.

## 19.7.2 Available recipes and diagnostics

Recipes are stored in recipes/

recipe\_runoff\_et.yml

Diagnostics are stored in diag\_scripts/runoff\_et/

• catchment\_analysis.py: bar and scatter plots for catchment averages of runoff, evapotranspiration and precipitation

## 19.7.3 User settings in recipe

1. Script catchment\_analysis.py

Required settings (scripts)

• catchmentmask: netCDF file indicating the grid cell for a specific catchment. Modus of distribution not yet clearified. ESGF?

Optional settings (variables)

• reference\_dataset: dataset\_name Datasets can be used as reference instead of defaults provided with the diagnostics. Must be identical for all variables.

# 19.7.4 Variables

- evspsbl (atmos, monthly mean, time latitude longitude)
- pr (atmos, monthly mean, time latitude longitude)
- mrro (land, monthly mean, time latitude longitude)

# 19.7.5 Observations and reformat scripts

Default reference data based on GRDC and WFDEI are included in the diagnostic script as catchment averages. They can be replaced with any gridded dataset by defining a reference\_dataset. The necessary catchment mask is available at

All other datasets are remapped onto the catchment mask grid as part of the diagnostics.

# 19.7.6 References

- Duemenil Gates, L., S. Hagemann and C. Golz, Observed historical discharge data from major rivers for climate model validation. Max Planck Institute for Meteorology Report 307, Hamburg, Germany, 2000.
- Hagemann, S., A. Loew, A. Andersson, Combined evaluation of MPI-ESM land surface water and energy fluxes J. Adv. Model. Earth Syst., 5, doi:10.1029/2012MS000173, 2013.
- Weedon, G. P., G. Balsamo, N. Bellouin, S. Gomes, M. J. Best, and P. Viterbo, The WFDEI meteorological forcing data set: WATCH Forcing Data methodology applied to ERA-Interim reanalysis data, Water Resour. Res., 50, 7505–7514, doi: 10.1002/2014WR015638, 2014

# 19.7.7 Example plots

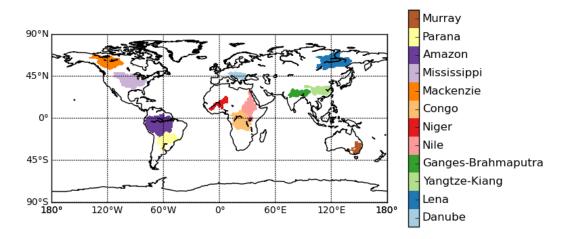


Fig. 20: Catchment definitions used in the diagnostics.

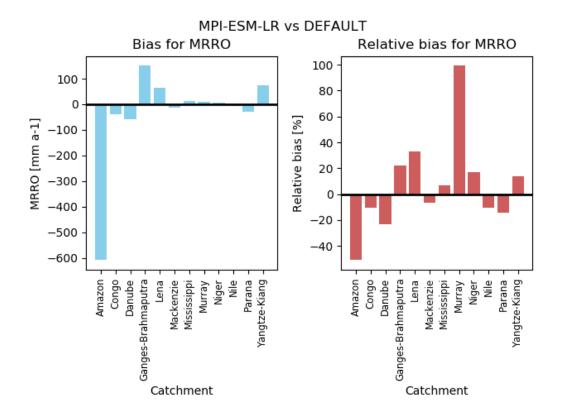


Fig. 21: Barplot indicating the absolute and relative bias in annual runoff between MPI-ESM-LR (1970-2000) and long term GRDC data for specific catchments.

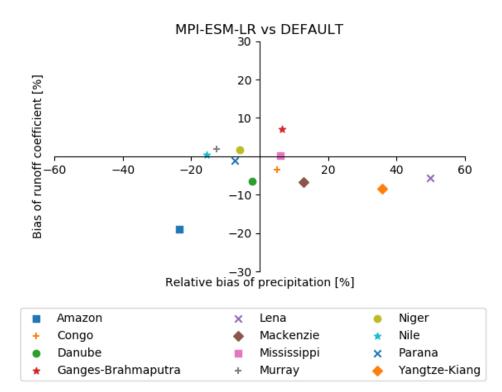


Fig. 22: Biases in runoff coefficient (runoff/precipitation) and precipitation for major catchments of the globe. The MPI-ESM-LR historical simulation (1970-2000) is used as an example.

## CHAPTER

# TWENTY

# OCEAN

# 20.1 Recipe for evaluating Arctic Ocean

### 20.1.1 Overview

The Arctic ocean is one of the areas of the Earth where the effects of climate change are especially visible today. Two most prominent processes are Arctic amplification [e.g. Serreze and Barry, 2011] and decrease of the sea ice area and thickness. Both receive good coverage in the literature and are already well-studied. Much less attention is paid to the interior of the Arctic Ocean itself. In order to increase our confidence in projections of the Arctic climate future proper representation of the Arctic Ocean hydrography is necessary.

The main focus of this diagnostics is evaluation of ocean components of climate models in the Arctic Ocean, however most of the diagnostics are implemented in a way that can be easily expanded to other parts of the World Ocean. Most of the diagnostics aim at model comparison to climatological data (PHC3), so we target historical CMIP simulations. However scenario runs also can be analysed to have an impression of how Arcti Ocean hydrography will chnage in the future.

At present only the subset of CMIP models can be used in particular because our analysis is limited to z coordinate models.

# 20.1.2 Available recipes

Recipe is stored in recipes/

• recipe\_arctic\_ocean.yml : contains all setting nessesary to run diagnostics and metrics.

Currenly the workflow do not allow to easily separate diagnostics from each other, since some of the diagnostics rely on the results of other diagnostics. The recipe currently do not use preprocessor options, so input files are CMORised monthly mean 3D ocean varibales on original grid.

The following plots will be produced by the recipe:

#### Hovmoeller diagrams

The characteristics of vertical TS distribution can change with time, and consequently the vertical TS distribution is an important indicator of the behaviour of the coupled ocean-sea ice-atmosphere system in the North Atlantic and Arctic Oceans. One way to evaluate these changes is by using Hovmoller diagrams. Hovmoller diagrams for two main Arctic Ocean basins – Eurasian and Amerasian with T and S spatially averaged on a monthly basis for every vertical level are available. This diagnostic allows the temporal evolution of vertical ocean potential temperature distribution to be assessed.

Related settings in the recipe:

	# Define regions, as a list.		
	# 'EB' - Eurasian Basin of the Arctic Ocean		
	# 'AB' - Amerasian Basin of the Arctic Ocean		
	# 'Barents_sea' - Barrents Sea		
	<pre># 'North_sea' - North Sea</pre>		
	<pre>hofm_regions: ["AB" , 'EB']</pre>		
	<pre># Define variables to use, should also be in "variables"</pre>		
	<pre># entry of your diagnostic</pre>		
	<pre>hofm_vars: ['thetao', 'so']</pre>		
	<pre># Maximum depth of Hovmoeller and vertical profiles</pre>		
	hofm_depth: 1500		
	# Define if Hovmoeller diagrams will be ploted.		
hofm_plot: True			
	<pre># Define colormap (as a list, same size as list with variables)</pre>		
	# Only cmaps from matplotlib and cmocean are supported.		
	<pre># Additional cmap - 'custom_salinity1'.</pre>		
	<pre>hofm_cmap: ['Spectral_r', 'custom_salinity1']</pre>		
	# Data limits for plots,		
	# List of the same size as the list of the variables		
	<pre># each entry is [vmin, vmax, number of levels, rounding limit]</pre>		
	hofm_limits: [[-2, 2.3, 41, 1], [30.5, 35.1, 47, 2]]		
	# Number of columns in the plot		
	hofm_ncol: 3		

#### **Vertical profiles**

The vertical structure of temperature and salinity (T and S) in the ocean model is a key diagnostic that is used for ocean model evaluation. Realistic T and S distributions means that model properly represent dynamic and thermodynamic processes in the ocean. Different ocean basins have different hydrological regimes so it is important to perform analysis of vertical TS distribution for different basins separately. The basic diagnostic in this sense is mean vertical profiles of temperature and salinity over some basin averaged for relatively long period of time. In addition to individual vertical profiles for every model, we also show the mean over all participating models and similar profile from climatological data (PHC3).

Several settings for vertical profiles (region, variables, maximum depths) will be determined by the Hovmoeller diagram settings. The reason is that vertical profiles are calculated from Hovmoeller diagram data. Mean vertical profile is calculated by linerally interpolating data on standard WOA/PHC depths.

Related settings in the recipe:

```
# Define regions, as a list.
# 'EB' - Eurasian Basin of the Arctic Ocean
# 'AB' - Amerasian Basin of the Arctic Ocean
```

(continues on next page)

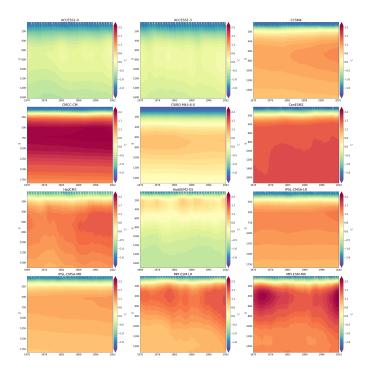


Fig. 1: Hovmoller diagram of monthly spatially averaged potential temperature in the Eurasian Basin of the Arctic Ocean for selected CMIP5 climate models (1970-2005).

```
(continued from previous page)
# 'Barents_sea' - Barrents Sea
# 'North_sea' - North Sea
hofm_regions: ["AB" , 'EB']
# Define variables to use, should also be in "variables" entry of your_
_ diagnostic
hofm_vars: ['thetao', 'so']
# Maximum depth of Hovmoeller and vertical profiles
hofm_depth: 1500
```

#### Spatial distribution maps of variables

The spatial distribution of basic oceanographic variables characterises the properties and spreading of ocean water masses. For the coupled models, capturing the spatial distribution of oceanographic variables is especially important in order to correctly represent the ocean-ice-atmosphere interface. We have implemented plots with spatial maps of temperature and salinity at original model levels.

Plots spatial distribution of variables at selected depths in North Polar projection on original model grid. For plotting the model depths that are closest to provided *plot2d\_depths* will be selected. Settings allow to define color maps and limits for each variable individually. Color maps should be ehter part of standard matplotlib set or one of the cmocean color maps. Additional colormap *custom\_salinity1* is provided.

Related settings in the recipe:

```
# Depths for spatial distribution maps
plot2d_depths: [10, 100]
# Variables to plot spatial distribution maps
```

(continues on next page)

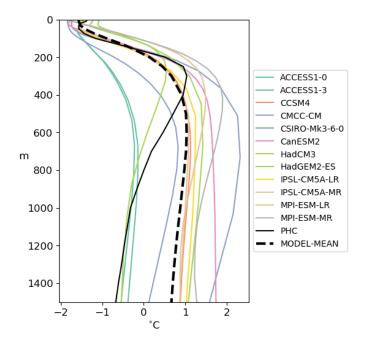


Fig. 2: Mean (1970-2005) vertical potential temperature distribution in the Eurasian basin for participating CMIP5 coupled ocean models, PHC3 climatology (dotted red line) and multi-model mean (dotted black line).

```
(continued from previous page)
plot2d_vars: ['thetao', 'so']
# Define colormap (as a list, same size as list with variables)
# Only cmaps from matplotlib and cmocean are supported.
# Additional cmap - 'custom_salinity1'.
plot2d_cmap: ['Spectral_r', 'custom_salinity1']
# Data limits for plots,
# List of the same size as the list of the variables
# each entry is [vmin, vmax, number of levels, rounding limit]
plot2d_limits: [[-2, 4, 20, 1], [30.5, 35.1, 47, 2]]
# number of columns for plots
plot2d_ncol: 3
```

#### Spatial distribution maps of biases

For temperature and salinity, we have implemented spatial maps of model biases from the observed climatology. For the model biases, values from the original model levels are linearly interpolated to the climatology and then spatially interpolated from the model grid to the regular PHC (climatology) grid. Resulting fields show model performance in simulating spatial distribution of temperature and salinity.

Related settings in the recipe:

```
plot2d_bias_depths: [10, 100]
# Variables to plot spatial distribution of the bias for.
plot2d_bias_vars: ['thetao', 'so']
# Color map names for every variable
plot2d_bias_cmap: ['balance', 'balance']
```

(continues on next page)

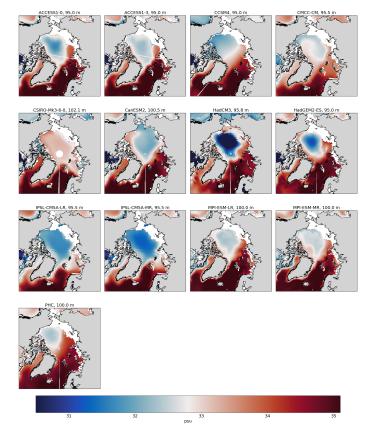


Fig. 3: Mean (1970-2005) salinity distribution at 100 meters.

(continued from previous page)

```
# Data limits for plots,
# List of the same size as the list of the variables
# each entry is [vmin, vmax, number of levels, rounding limit]
plot2d_bias_limits: [[-3, 3, 20, 1], [-2, 2, 47, 2]]
# number of columns in the bias plots
plot2d_bias_ncol: 3
```

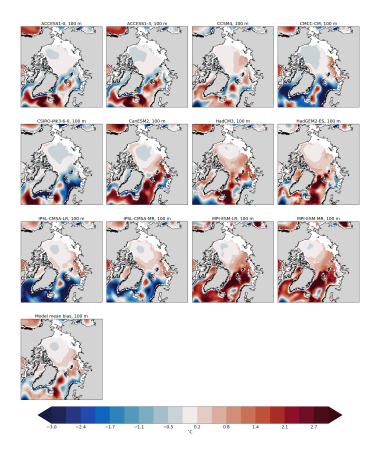


Fig. 4: Mean (1970-2005) salinity bias at 100m relative to PHC3 climatology

#### Transects

Vertical transects through arbitrary sections are important for analysis of vertical distribution of ocean water properties and especially useful when exchange between different ocean basins is evaluated. We have implemented diagnostics that allow for the definition of an arbitrary ocean section by providing set of points on the ocean surface. For each point, a vertical profile on the original model levels is interpolated. All profiles are then connected to form a transect. The great-circle distance between the points is calculated and used as along-track distance.

One of the main use cases is to create vertical sections across ocean passages, for example Fram Strait.

Plots transect maps for pre-defined set of transects (defined in *regions.py*, see below). The *transect\_depth* defines maximum depth of the transect. Transects are calculated from data averaged over the whole time period.

Related settings in the recipe:

```
# Select regions (transects) to plot
# Available options are:
# AWpath - transect along the path of the Atlantic Water
# Fram - Fram strait
transects_regions: ["AWpath", "Fram"]
# Variables to plot on transects
transects_vars: ['thetao', 'so']
# Color maps for every variable
transects_cmap: ['Spectral_r', 'custom_salinity1']
# Data limits for plots,
# List of the same size as the list of the variables
# each entry is [vmin, vmax, number of levels, rounding limit]
transects_limits: [[-2, 4, 20, 1], [30.5, 35.1, 47, 2]]
# Maximum depth to plot the data
transects_depth: 1500
# number of columns
transects_ncol: 3
```

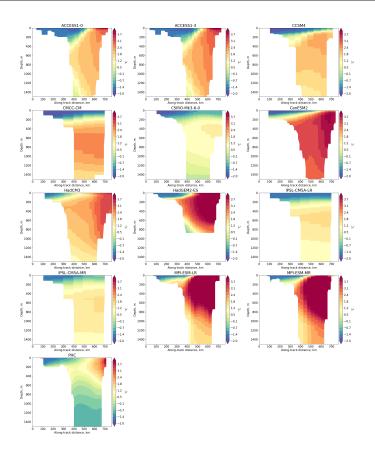


Fig. 5: Mean (1970-2005) potential temperature across the Fram strait.

#### Atlantic Water core depth and temperature

Atlantic water is a key water mass of the Arctic Ocean and its proper representation is one of the main challenges in Arctic Ocean modelling. We have created two metrics by which models can be easily compared in terms of Atlantic water simulation. The temperature of the Atlantic Water core is calculated for every model as the maximum potential temperature between 200 and 1000 meters depth in the Eurasian Basin. The depth of the Atlantic Water core is calculated as the model level depth where the maximum temperature is found in Eurasian Basin (Atlantic water core temperature).

The AW core depth and temperature will be calculated from data generated for Hovmoeller diagrams for *EB* region, so it should be selected in the Hovmoeller diagrams settings as one of the *hofm\_regions*.

In order to evaluate the spatial distribution of Atlantic water in different climate models we also provide diagnostics with maps of the spatial temperature distribution at model's Atlantic Water depth.

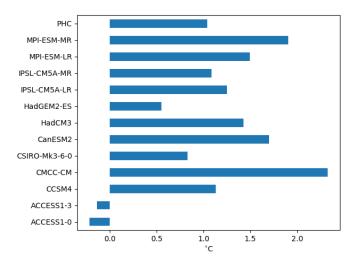


Fig. 6: Mean (1970-2005) Atlantic Water core temperature. PHC33 is an observed climatology.

#### **TS-diagrams**

T-S diagrams combine temperature and salinity, which allows the analysis of water masses and their potential for mixing. The lines of constant density for specific ranges of temperature and salinity are shown on the background of the T-S diagram. The dots on the diagram are individual grid points from specified region at all model levels within user specified depth range.

Related settings in the recipe:

```
tsdiag_regions: ["AB" , 'EB']
# Maximum depth to consider data for TS diagrams
tsdiag_depth: 1500
# Number of columns
tsdiag_ncol: 3
```

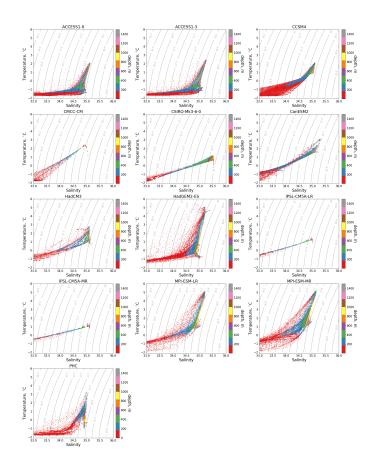


Fig. 7: Mean (1970-2005) T-S diagrams for Eurasian Basin of the Arctic Ocean.

# 20.1.3 Available diagnostics

The following python modules are included in the diagnostics package:

- arctic\_ocean.py : Reads settings from the recipe and call functions to do analysis and plots.
- getdata.py : Deals with data preparation.
- interpolation.py : Include horizontal and vertical interpolation functions specific for ocean models.
- plotting.py : Ocean specific plotting functions
- regions.py : Contains code to select specific regions, and definition of the regions themselves.
- utils.py : Helpful utilites.

Diagnostics are stored in diag\_scripts/arctic\_ocean/

#### Variables

- thetao (ocean, monthly, longitude, latitude, time)
- so (ocean, monthly, longitude, latitude, time)

#### **Observations and reformat scripts**

• PHC3 climatology

#### References

- Ilicak, M. et al., An assessment of the Arctic Ocean in a suite of interannual CORE-II simulations. Part III: Hydrography and fluxes, Ocean Modelling, Volume 100, April 2016, Pages 141-161, ISSN 1463-5003, doi.org/10.1016/j.ocemod.2016.02.004
- Steele, M., Morley, R., & Ermold, W. (2001). PHC: A global ocean hydrography with a high-quality Arctic Ocean. Journal of Climate, 14(9), 2079-2087.
- Wang, Q., et al., An assessment of the Arctic Ocean in a suite of interannual CORE-II simulations. Part I: Sea ice and solid freshwater, Ocean Modelling, Volume 99, March 2016, Pages 110-132, ISSN 1463-5003, doi.org/10.1016/j.ocemod.2015.12.008
- Wang, Q., Ilicak, M., Gerdes, R., Drange, H., Aksenov, Y., Bailey, D. A., ... & Cassou, C. (2016). An assessment of the Arctic Ocean in a suite of interannual CORE-II simulations. Part II: Liquid freshwater. Ocean Modelling, 99, 86-109, doi.org/10.1016/j.ocemod.2015.12.009

# 20.2 Climate Variability Diagnostics Package (CVDP)

### 20.2.1 Overview

The Climate Variability Diagnostics Package (CVDP) developed by NCAR's Climate Analysis Section is an analysis tool that documents the major modes of climate variability in models and observations, including ENSO, Pacific Decadal Oscillation, Atlantic Multi-decadal Oscillation, Northern and Southern Annular Modes, North Atlantic Oscillation, Pacific North and South American teleconnection patterns. For details please refer to the [1] and [2].

## 20.2.2 Available recipes and diagnostics

Recipes are stored in recipes/

recipe\_cvdp.yml

Diagnostics are stored in diag\_scripts/cvdp/

• cvdp\_wrapper.py

# 20.2.3 User settings in recipe

The recipe can be run with several data sets including different model ensembles, multi-model mean statistics are currently not supported.

# 20.2.4 Variables

- ts (atmos, monthly mean, longitude latitude time)
- tas (atmos, monthly mean, longitude latitude time)
- pr (atmos, monthly mean, longitude latitude time)
- psl (atmos, monthly mean, longitude latitude time)

# 20.2.5 Observations and reformat scripts

None.

# 20.2.6 References

[1] http://www.cesm.ucar.edu/working\_groups/CVC/cvdp/

[2] https://github.com/NCAR/CVDP-ncl

# 20.2.7 Example plots

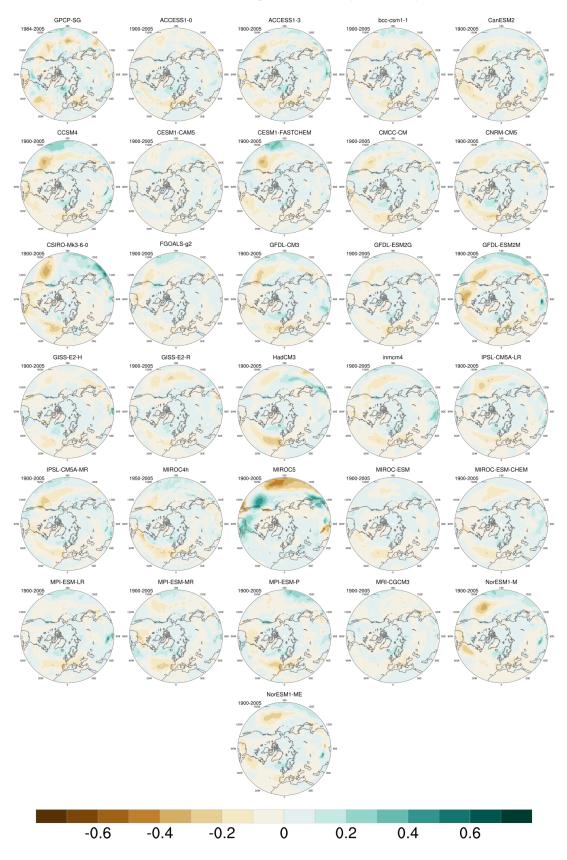
# 20.3 Nino indices, North Atlantic Oscillation (NAO), Souther Oscillation Index (SOI)

### 20.3.1 Overview

The goal of this diagnostic is to compute indices based on area averages.

In recipe\_combined\_indices.yml, after defining the period (historical or future projection), the variable is selected. The predefined areas are:

- Nino 3
- Nino 3.4
- Nino 4
- North Atlantic Oscillation (NAO)



NAM PR Regressions (Annual)

Fig. 8: Regression of the precipitation anomalies (PR) onto the Northern Annular Mode (NAM) index for the time period 1900-2005 for 30 CMIP5 models and observations (GPCP (pr) / IFS-Cy31r2 (psl); time period 1984-2005).

• Southern Oscillation Index (SOI)

## 20.3.2 Available recipes and diagnostics

Recipes are stored in recipes/

• recipe\_combined\_indices.yml

Diagnostics are stored in diag\_scripts/magic\_bsc/

• combined\_indices.R : calculates the area-weighted means and multi-model means, with or without weights

## 20.3.3 User settings

User setting files are stored in recipes/

1. recipe\_combined\_indices.yml

Required settings for script

- region: one of the following strings Nino3, Nino3.4, Nino4, NAO, SOI
- running\_mean: an integer specifying the length of the window (in months) to be used for computing the running mean.
- moninf: an integer can be given to determine the first month of the seasonal mean to be computed (from 1 to 12, corresponding to January to December respectively).
- monsup: an integer specifying the last month to be computed (from 1 to 12, corresponding to January to December respectively).
- standardized: 'true' or 'false' to specify whether to compute the standarization of the variable.

Required settings for preprocessor (only for 3D variables)

extract\_levels:

- levels: [50000] # e.g. for 500 hPa level
- scheme: nearest

### 20.3.4 Variables

• all variables (atmos/ocean, monthly, longitude, latitude, time)

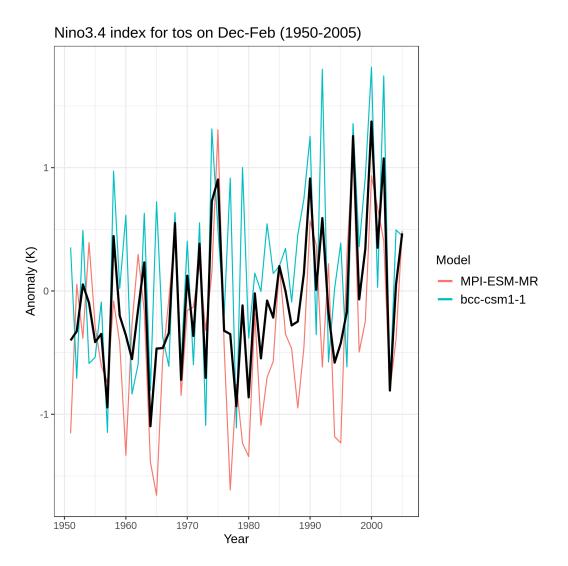
### 20.3.5 Observations and reformat scripts

None

## 20.3.6 References

• Trenberth, Kevin & National Center for Atmospheric Research Staff (Eds). Last modified 11 Jan 2019. "The Climate Data Guide: Nino SST Indices (Nino 1+2, 3, 3.4, 4; ONI and TNI)." Retrieved from https: //climatedataguide.ucar.edu/climate-data/nino-sst-indices-nino-12-3-34-4-oni-and-tni.

# 20.3.7 Example plots



Time series of the standardized sea surface temperature (tos) area averaged over the Nino 3.4 region during the boreal winter (December-January-February). The time series correspond to the MPI-ESM-MR (red) and BCC-CSM1-1 (blue) models and their mean (black) during the period 1950-2005 for the ensemble r1p1i1 of the historical simulations.

# 20.4 Ocean chlorophyll in ESMs compared to ESA-CCI observations.

## 20.4.1 Overview

This recipe compares monthly surface chlorophyll from CMIP models to ESA CCI ocean colour chlorophyll (ESACCI-OC). The observations are the merged sensor geographic monthly L3S chlor\_a data Sathyendranath et al. (2019). Multiple models and different observational versions can be used by the script.

The recipe\_esacci\_oc.yml produces an image showing four maps. Each of these four maps shows latitude vs longitude and the chlorophyll value. The four plots are: ESACCI-OC v5.0 chlorophyll, the CMIP6 model, the bias model-observation and the ratio model/observations. The script also produces a scatter plot for all coordinates with the model on the x-axis and the observations on the y axis and a line of best fit with the parameter values given in the panel.

# 20.4.2 Available recipes and diagnostics

Recipes are stored in esmvaltool/recipes/ocean/

recipe\_esacci\_oc.yml

Diagnostics are stored in esmvaltool/diag\_scripts/ocean/

diagnostic\_model\_vs\_obs.py

## 20.4.3 User settings in recipe

1. Script diagnostic\_model\_vs\_obs.py

Required settings for script

• observational\_dataset: name of reference dataset (e.g. {dataset: ESACCI-OC,})

# 20.4.4 Variables

• chl (ocean, monthly mean, longitude, latitude, time)

### 20.4.5 Observations and reformat scripts

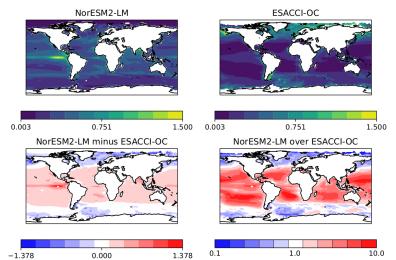
• ESACCI-OC (chl)

Reformat script: reformat\_scripts/obs/reformat\_obs\_esacci\_oc.py

# 20.4.6 References

- Sathyendranath, S., et al. (2019), An ocean-colour time series for use in climate studies: the experience of the Ocean-Colour Climate Change Initiative (OC-CCI). Sensors: 19, 4285. doi:10.3390/s19194285.
- ESACCI-OC dataset: http://dx.doi.org/10.5285/00b5fc99f9384782976a4453b0148f49

## 20.4.7 Example plots



Mass Concentration of Total Phytoplankton Expressed as Chlorophyll in Sea Water [mg m-3]

Fig. 9: Surface chlorophyll from ESACCI-OC ocean colour data version 5.0 and the CMIP6 model NorESM2-LM. This model overestimates chlorophyll compared to the observations.

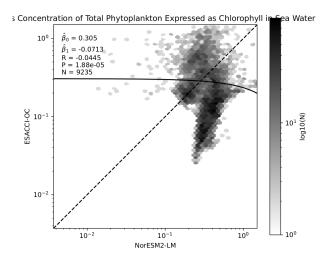


Fig. 10: Scatter plot of surface chlorophyll from ESACCI-OC ocean colour data version 5.0 and the CMIP6 model NorESM2-LM.

# 20.5 Ocean diagnostics

#### 20.5.1 Overview

These recipes are used for evaluating the marine component of models of the earth system. Using these recipes, it should be possible to evaluate both the physical models and biogeochemistry models. All these recipes use the ocean diagnostics package.

The ocean diagnostics package contains several diagnostics which produce figures and statistical information of models of the ocean. The datasets have been pre-processed by ESMValTool, based on recipes in the recipes directory. Most of

the diagnostics produce two or less types of figure, and several diagnostics are called by multiple recipes.

Each diagnostic script expects a metadata file, automatically generated by ESMValTool, and one or more pre-processed dataset. These are passed to the diagnostic by ESMValTool in the settings.yml and metadata.yml files.

The ocean diagnostics toolkit can not figure out how to plot data by itself. The current version requires the recipe to produce the correct pre-processed data for each diagnostic script. ie: to produce a time series plot, the preprocessor must produce a time-dimensional dataset.

While these tools were built to evaluate the ocean component models, they also can be used to produce figures for other domains. However, there are some ocean specific elements, such as the z-direction being positive and reversed, and some of the map plots have the continents coloured in by default.

As elsewhere, both the model and observational datasets need to be compliant with the CMOR data.

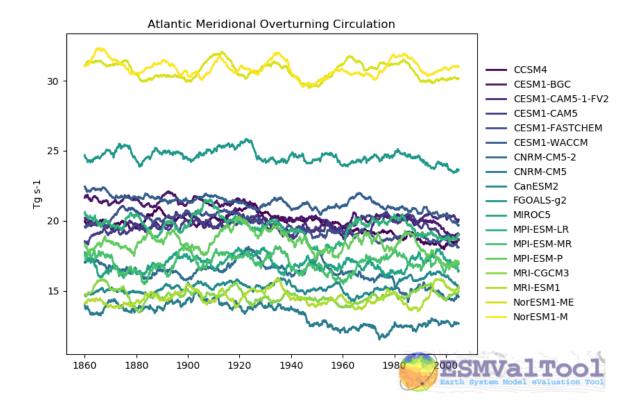
## 20.5.2 Available recipes

- recipe\_ocean\_amoc.yml
- recipe\_ocean\_example.yml
- recipe\_ocean\_scalar\_fields.yml
- recipe\_ocean\_bgc.yml
- recipe\_ocean\_quadmap.yml
- recipe\_ocean\_ice\_extent.yml
- recipe\_ocean\_multimap.yml

#### recipe\_ocean\_amoc.yml

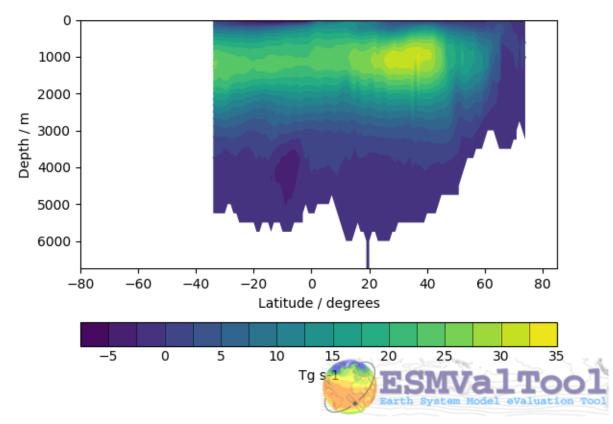
The recipe\_ocean\_amoc.yml is an recipe that produces figures describing the Atlantic Meridional Overturning Circulation (AMOC) and the drake passage current.

The recipes produces time series of the AMOC at 26 north and the drake passage current.

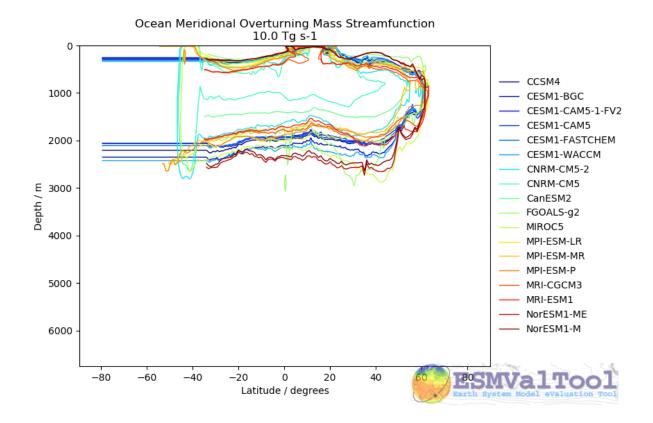


This figure shows the multi model comparison of the AMOC from several CMIP5 historical simulations, with a 6 year moving average (3 years either side of the central value). A similar figure is produced for each individual model, and for the Drake Passage current.

This recipe also produces a contour transect and a coloured transect plot showing the Atlantic stream function for each individual model, and a multi-model contour is also produced:



NorESM1-M Ocean Meridional Overturning Mass Streamfunction



#### recipe\_ocean\_example.yml

The recipe\_ocean\_example.yml is an example recipe which shows several examples of how to manipulate marine model data using the ocean diagnostics tools.

While several of the diagnostics here have specific uses in evaluating models, it is meant to be a catch-all recipe demonstrating many different ways to evaluate models.

All example calculations are performed using the ocean temperature in a three dimensional field (thetao), or at the surface (tos). This recipe demonstrates the use of a range of preprocessors in a marine context, and also shows many of the standard model-only diagnostics (no observational component is included.)

This recipe includes examples of how to manipulate both 2D and 3D fields to produce:

- Time series:
  - Global surface area weighted mean time series
  - Volume weighted average time series within a specific depth range
  - Area weighted average time series at a specific depth
  - Area weighted average time series at a specific depth in a specific region.
  - Global volume weighted average time series
  - Regional volume weighted average time series
- Maps:
  - Global surface map (from 2D ad 3D initial fields)

- Global surface map using re-gridding to a regular grid
- Global map using re-gridding to a regular grid at a specific depth level
- Regional map using re-gridding to a regular grid at a specific depth level
- Transects:
  - Produce various transect figure showing a re-gridded transect plot, and multi model comparisons
- Profile:
  - Produce a Global area-weighted depth profile figure
  - Produce a regional area-weighted depth profile figure

All the these fields can be expanded using a

#### recipe\_ocean\_bgc.yml

The recipe\_ocean\_bgc.yml is an example recipe which shows a several simple examples of how to manipulate marine biogeochemical model data.

This recipe includes the following fields:

- Global total volume-weighted average time series:
  - temperature, salinity, nitrate, oxygen, silicate (vs WOA data) \*
  - chlorophyll, iron, total alkalinity (no observations)
- Surface area-weighted average time series:
  - temperature, salinity, nitrate, oxygen, silicate (vs WOA data) \*
  - fgco2 (global total), integrated primary production, chlorophyll, iron, total alkalinity (no observations)
- Scalar fields time series:
  - mfo (including stuff like drake passage)
- Profiles:
  - temperature, salinity, nitrate, oxygen, silicate (vs WOA data) \*
  - chlorophyll, iron, total alkalinity (no observations)
- Maps + contours:
  - temperature, salinity, nitrate, oxygen, silicate (vs WOA data) \*
  - chlorophyll, iron, total alkalinity (no observations)
- Transects + contours:
  - temperature, salinity, nitrate, oxygen, silicate (vs WOA data) \*
  - chlorophyll, iron, no observations)

\* Note that Phosphate is also available as a WOA diagnostic, but I haven't included it as HadGEM2-ES doesn't include a phosphate field.

This recipe uses the World Ocean Atlas data, which can be downloaded from: https://www.ncei.noaa.gov/products/ world-ocean-atlas (last access 02/08/2021)

Instructions: Select the "All fields data links (1° grid)" netCDF file, which contain all fields.

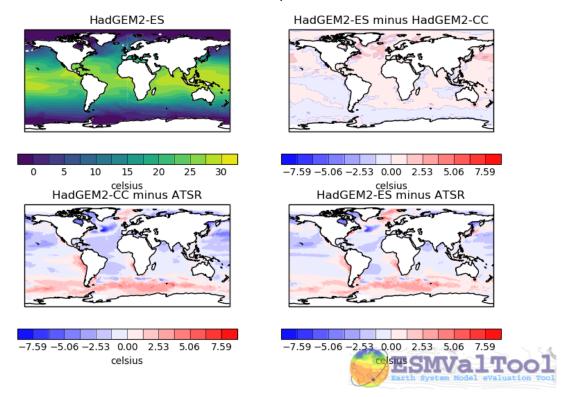
#### recipe\_ocean\_quadmap.yml

The recipe\_ocean\_quadmap.yml is an example recipe showing the diagnostic\_maps\_quad.py diagnostic. This diagnostic produces an image showing four maps. Each of these four maps show latitude vs longitude and the cube value is used as the colour scale. The four plots are:

model1	model 1 minus model2
model2 minus obs	model1 minus obs

These figures are also known as Model vs Model vs Obs plots.

The figure produced by this recipe compares two versions of the HadGEM2 model against ATSR sea surface temperature:



#### Sea Surface Temperature

This kind of figure can be very useful when developing a model, as it allows model developers to quickly see the impact of recent changes to the model.

#### recipe ocean ice extent.yml

The *recipe\_ocean\_ice\_extent.yml* recipe produces several metrics describing the behaviour of sea ice in a model, or in multiple models.

This recipe has four preprocessors, a combinatorial combination of

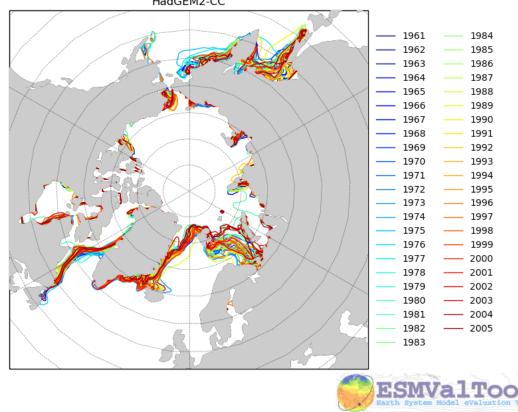
- Regions: Northern or Southern Hemisphere
- · Seasons: December-January-February or June-July-August

Once these seasonal hemispherical fractional ice cover is processed, the resulting cube is passed 'as is' to the diagnostic\_seaice.py diagnostic.

This diagnostic produces the plots:

- Polar Stereographic projection Extent plots of individual models years.
- Polar Stereographic projection maps of the ice cover and ice extent for individual models.
- A time series of Polar Stereographic projection Extent plots see below.
- Time series plots of the total ice area and the total ice extent.

The following image shows an example of the sea ice extent plot, showing the Summer Northern hemisphere ice extent for the HadGEM2-CC model, in the historical scenario.



The sea ice diagnostic is unlike the other diagnostics in the ocean diagnostics toolkit. The other tools are build to be generic plotting tools which work with any field (ie diagnostic\_timeseries.py works fine for Temperature,

HadGEM2-CC

Chlorophyll, or any other field. On the other hand, the sea ice diagnostic is the only tool that performs a field specific evaluation.

The diagnostic\_seaice.py diagnostic is more fully described below.

#### recipe\_ocean\_multimap.yml

The recipe\_ocean\_multimap.yml is an example recipe showing the diagnostic\_maps\_multimodel.py diagnostic. This diagnostic produces an image showing Model vs Observations maps or only Model fields when observational data are not provided. Each map shows latitude vs longitude fields and user defined values are used to set the colour scale. Plot layout can be modified by modifying the *layout\_rowcol* argument.

The figure produced by this recipe compares the ocean surface CO2 fluxes for 16 different CMIP5 model against Landschuetzer2016 observations.

The diagnostic\_maps\_multimodel.py diagnostic is documented below.

#### 20.5.3 Available diagnostics

Diagnostics are stored in the diag\_scripts directory: ocean.

The following python modules are included in the ocean diagnostics package. Each module is described in more detail both below and inside the module.

- diagnostic\_maps.py
- diagnostic\_maps\_quad.py
- diagnostic\_model\_vs\_obs.py
- diagnostic\_profiles.py
- diagnostic\_seaice.py
- diagnostic\_timeseries.py
- diagnostic\_tools.py
- diagnostic\_transects.py
- diagnostic\_maps\_multimodel.py

#### diagnostic\_maps.py

The diagnostic\_maps.py produces a spatial map from a NetCDF. It requires the input netCDF to have the following dimensions. Either:

- A two dimensional file: latitude, longitude.
- A three dimensional file: depth, latitude, longitude.

In the case of a 3D netCDF file, this diagnostic produces a map for EVERY layer. For this reason, we recommend extracting a small number of specific layers in the preprocessor, using the *extract\_layer* preprocessor.

This script can not process NetCDFs with multiple time steps. Please use the *climate\_statistics* preprocessor to collapse the time dimension.

This diagnostic also includes the optional arguments, threshold and thresholds.

- threshold: a single float.
- thresholds: a list of floats.

Only one of these arguments should be provided at a time. These two arguments produce a second kind of diagnostic map plot: a contour map showing the spatial distribution of the threshold value, for each dataset. Alternatively, if the thresholds argument is used instead of threshold, the single-dataset contour map shows the contours of all the values in the thresholds list.

If multiple datasets are provided, in addition to the single dataset contour, a multi-dataset contour map is also produced for each value in the thresholds list.

Some appropriate preprocessors for this diagnostic would be:

For a Global 2D field:

```
prep_map_1:
    climate_statistics:
```

For a regional 2D field:

```
prep_map_2:
    extract_region:
        start_longitude: -80.
        end_longitude: 30.
        start_latitude: -80.
        end_latitude: 80.
climate_statistics:
        operator: mean
```

For a Global 3D field at the surface and 10m depth:

```
prep_map_3:
    custom_order: true
    extract_levels:
        levels: [0., 10.]
        scheme: linear_horizontal_extrapolate_vertical
climate_statistics:
    operator: mean
```

For a multi-model comparison mean of 2D global fields including contour thresholds.

```
prep_map_4:
    custom_order: true
climate_statistics:
    operator: mean
    regrid:
       target_grid: 1x1
       scheme: linear
```

And this also requires the threshold key in the diagnostic:

```
diagnostic_map:
  variables:
    tos: # Temperature ocean surface
        preprocessor: prep_map_4
        field: TO2M
    scripts:
        Ocean_regrid_map:
```

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script: ocean/diagnostic\_maps.py
thresholds: [5, 10, 15, 20]

#### diagnostic\_maps\_quad.py

The diagnostic\_maps\_quad.py diagnostic produces an image showing four maps. Each of these four maps show latitude vs longitude and the cube value is used as the colour scale. The four plots are:

model1	model 1 minus model2
model2 minus obs	model1 minus obs

These figures are also known as Model vs Model vs Obs plots.

This diagnostic assumes that the preprocessors do the bulk of the hard work, and that the cubes received by this diagnostic (via the settings.yml and metadata.yml files) have no time component, a small number of depth layers, and a latitude and longitude coordinates.

An appropriate preprocessor for a 2D field would be:

and an example of an appropriate diagnostic section of the recipe would be:

```
diag_map_1:
 variables:
   tos: # Temperature ocean surface
     preprocessor: prep_quad_map
      field: TO2Ms
     mip: Omon
 additional_datasets:
         filename: tos_ATSR_L3_ARC-v1.1.1_199701-201112.nc
#
         download from: https://datashare.is.ed.ac.uk/handle/10283/536
#
    - {dataset: ATSR, project: obs4MIPs, level: L3, version: ARC-v1.1.1,

start_year: 2001, end_year: 2003, tier: 3}

 scripts:
   Global_Ocean_map:
      script: ocean/diagnostic_maps_quad.py
      control_model: {dataset: HadGEM2-CC, project: CMIP5, mip: Omon, exp:_
→historical. ensemble: r1i1p1}
      exper_model: {dataset: HadGEM2-ES, project: CMIP5, mip: Omon, exp:_
→historical. ensemble: r1i1p1}
      observational_dataset: {dataset: ATSR, project: obs4MIPs,}
```

Note that the details about the control model, the experiment models and the observational dataset are all provided in the script section of the recipe.

#### diagnostic\_model\_vs\_obs.py

The diagnostic\_model\_vs\_obs.py diagnostic makes model vs observations maps and scatter plots. The map plots shows four latitude vs longitude maps:

Model	Observations
Model minus Observations	Model over Observations

Note that this diagnostic assumes that the preprocessors do the bulk of the hard work, and that the cube received by this diagnostic (via the settings.yml and metadata.yml files) has no time component, a small number of depth layers, and a latitude and longitude coordinates.

This diagnostic also includes the optional arguments, *maps\_range* and *diff\_range* to manually define plot ranges. Both arguments are a list of two floats to set plot range minimun and maximum values respectively for Model and Observations maps (Top panels) and for the Model minus Observations panel (bottom left). Note that if input data have negative values the Model over Observations map (bottom right) is not produced.

The scatter plots plot the matched model coordinate on the x axis, and the observational dataset on the y coordinate, then performs a linear regression of those data and plots the line of best fit on the plot. The parameters of the fit are also shown on the figure.

An appropriate preprocessor for a 3D+time field would be:

```
preprocessors:
    prep_map:
    extract_levels:
        levels: [100., ]
        scheme: linear_extrap
climate_statistics:
    operator: mean
    regrid:
        target_grid: 1x1
        scheme: linear
```

#### diagnostic\_maps\_multimodel.py

The diagnostic\_maps\_multimodel.py diagnostic makes model(s) vs observations maps and if data are not provided it draws only model field.

It is always nessary to define the overall layout trough the argument *layout\_rowcol*, which is a list of two integers indicating respectively the number of rows and columns to organize the plot. Observations has not be accounted in here as they are automatically added at the top of the figure.

This diagnostic also includes the optional arguments, *maps\_range* and *diff\_range* to manually define plot ranges. Both arguments are a list of two floats to set plot range minimun and maximum values respectively for variable data and the Model minus Observations range.

Note that this diagnostic assumes that the preprocessors do the bulk of the hard work, and that the cube received by this diagnostic (via the settings.yml and metadata.yml files) has no time component, a small number of depth layers, and a latitude and longitude coordinates.

An appropriate preprocessor for a 3D+time field would be:

```
preprocessors:
    prep_map:
```

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```
extract_levels:
    levels: [100., ]
    scheme: linear_extrap
climate_statistics:
    operator: mean
    regrid:
    target_grid: 1x1
    scheme: linear
```

#### diagnostic\_profiles.py

The diagnostic\_profiles.py diagnostic produces images of the profile over time from a cube. These plots show cube value (ie temperature) on the x-axis, and depth/height on the y axis. The colour scale is the annual mean of the cube data. Note that this diagnostic assumes that the preprocessors do the bulk of the hard work, and that the cube received by this diagnostic (via the settings.yml and metadata.yml files) has a time component, and depth component, but no latitude or longitude coordinates.

An appropriate preprocessor for a 3D+time field would be:

```
preprocessors:
    prep_profile:
    extract_volume:
    long1: 0.
    long2: 20.
    lat1: -30.
    lat2: 30.
    z_min: 0.
    z_max: 3000.
    area_statistics:
    operator: mean
```

#### diagnostic\_timeseries.py

The diagnostic\_timeseries.py diagnostic produces images of the time development of a metric from a cube. These plots show time on the x-axis and cube value (ie temperature) on the y-axis.

Two types of plots are produced: individual model timeseries plots and multi model time series plots. The individual plots show the results from a single cube, even if this cube is a multi-model mean made by the *multimodel* preprocessor.

The multi model time series plots show several models on the same axes, where each model is represented by a different line colour. The line colours are determined by the number of models, their alphabetical order and the *jet* colour scale. Observational datasets and multimodel means are shown as black lines.

This diagnostic assumes that the preprocessors do the bulk of the work, and that the cube received by this diagnostic (via the settings.yml and metadata.yml files) is time-dimensional cube. This means that the pre-processed netcdf has a time component, no depth component, and no latitude or longitude coordinates.

Some appropriate preprocessors would be :

For a global area-weighted average 2D field:

```
area_statistics:
operator: mean
```

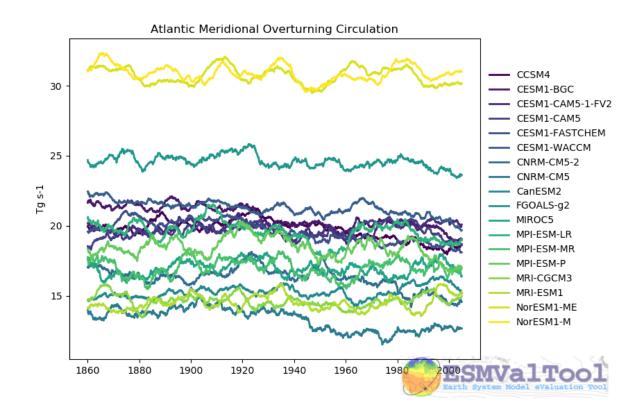
For a global volume-weighted average 3D field:

```
volume_statistics:
    operator: mean
```

For a global area-weighted surface of a 3D field:

```
extract_levels:
   levels: [0., ]
   scheme: linear_horizontal_extrapolate_vertical
   area_statistics:
    operator: mean
```

An example of the multi-model time series plots can seen here:



#### diagnostic\_transects.py

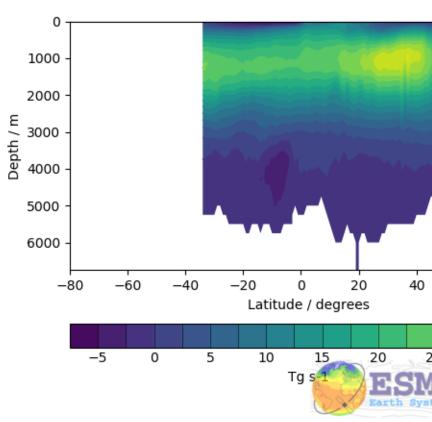
The diagnostic\_transects.py diagnostic produces images of a transect, typically along a constant latitude or longitude.

These plots show 2D plots with either latitude or longitude along the x-axis, depth along the y-axis and and the cube value is used as the colour scale.

This diagnostic assumes that the preprocessors do the bulk of the hard work, and that the cube received by this diagnostic (via the settings.yml and metadata.yml files) has no time component, and one of the latitude or longitude coordinates has been reduced to a single value.

An appropriate preprocessor for a 3D+time field would be:

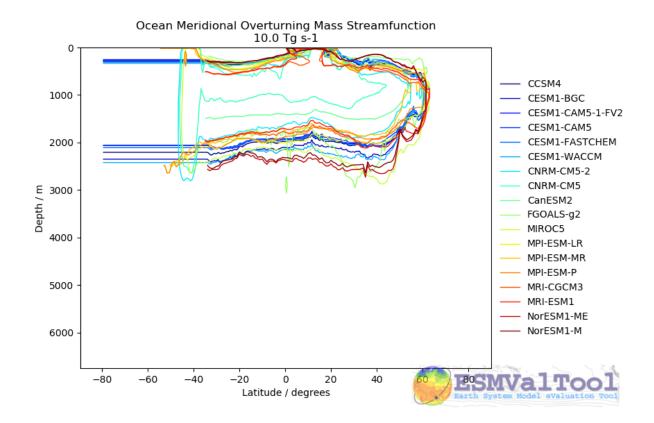
```
climate_statistics:
    operator: mean
extract_slice:
    latitude: [-50.,50.]
    longitude: 332.
```



## NorESM1-M Ocean Meridional Overturning Mass

Here is an example of the transect figure: .. centered::

And here is an example of the multi-model transect contour figure:



#### diagnostic\_seaice.py

The diagnostic\_seaice.py diagnostic is unique in this module, as it produces several different kinds of images, including time series, maps, and contours. It is a good example of a diagnostic where the preprocessor does very little work, and the diagnostic does a lot of the hard work.

This was done purposely, firstly to demonstrate the flexibility of ESMValTool, and secondly because Sea Ice is a unique field where several Metrics can be calculated from the sea ice cover fraction.

The recipe Associated with with diagnostic is the recipe\_SeaIceExtent.yml. This recipe contains 4 preprocessors which all perform approximately the same calculation. All four preprocessors extract a season: - December, January and February (DJF) - June, July and August (JJA) and they also extract either the North or South hemisphere. The four preprocessors are combinations of DJF or JJA and North or South hemisphere.

One of the four preprocessors is North Hemisphere Winter ice extent:

```
timeseries_NHW_ice_extent: # North Hemisphere Winter ice_extent
custom_order: true
extract_time: &time_anchor # declare time here.
    start_year: 1960
    start_month: 12
    start_day: 1
    end_year: 2005
    end_month: 9
    end_day: 31
extract_season:
    season: DJF
```

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```
extract_region:
   start_longitude: -180.
   end_longitude: 180.
   start_latitude: 0.
   end_latitude: 90.
```

Note that the default settings for ESMValTool assume that the year starts on the first of January. This causes a problem for this preprocessor, as the first DJF season would not include the first Month, December, and the final would not include both January and February. For this reason, we also add the *extract\_time* preprocessor.

This preprocessor group produces a 2D field with a time component, allowing the diagnostic to investigate the time development of the sea ice extend.

The diagnostic section of the recipe should look like this:

```
diag_ice_NHW:
    description: North Hemisphere Winter Sea Ice diagnostics
    variables:
    sic: # surface ice cover
        preprocessor: timeseries_NHW_ice_extent
        field: TO2M
        mip: OImon
    scripts:
    Global_seaice_timeseries:
        script: ocean/diagnostic_seaice.py
        threshold: 15.
```

Note the threshold here is 15%, which is the standard cut of for the ice extent.

The sea ice diagnostic script produces three kinds of plots, using the methods:

- make\_map\_extent\_plots: extent maps plots of individual models using a Polar Stereographic project.
- make\_map\_plots: maps plots of individual models using a Polar Stereographic project.
- make\_ts\_plots: time series plots of individual models

There are no multi model comparisons included here (yet).

#### diagnostic\_tools.py

The diagnostic\_tools.py is a module that contains several python tools used by the ocean diagnostics tools.

These tools are:

- folder: produces a directory at the path provided and returns a string.
- get\_input\_files: loads a dictionary from the input files in the metadata.yml.
- bgc\_units: converts to sensible units where appropriate (ie Celsius, mmol/m3)
- timecoord\_to\_float: Converts time series to decimal time ie: Midnight on January 1st 1970 is 1970.0
- add\_legend\_outside\_right: a plotting tool, which adds a legend outside the axes.
- get\_image\_format: loads the image format, as defined in the global user config.yml.
- get\_image\_path: creates a path for an image output.
- make\_cube\_layer\_dict: makes a dictionary for several layers of a cube.

We just show a simple description here, each individual function is more fully documented in the diagnostic\_tools.py module.

#### 20.5.4 A note on the auxiliary data directory

Some of these diagnostic scripts may not function on machines with no access to the internet, as cartopy may try to download the shape files. The solution to this issue is the put the relevant cartopy shapefiles in a directory which is visible to esmvaltool, then link that path to ESMValTool via the *auxiliary\_data\_dir* variable in your config-user.yml file.

The cartopy masking files can be downloaded from: https://www.naturalearthdata.com/downloads/

In these recipes, cartopy uses the 1:10, physical coastlines and land files:

```
110m_coastline.dbf
110m_coastline.shp
110m_coastline.shx
110m_land.dbf
110m_land.shp
110m_land.shx
```

#### 20.5.5 Associated Observational datasets

The following observations datasets are used by these recipes:

#### World Ocean ATLAS

These data can be downloaded from: https://www.nodc.noaa.gov/OC5/woa13/woa13data.html (last access 10/25/2018) Select the "All fields data links (1° grid)" netCDF file, which contain all fields.

#### The following WOA datasets are used by the ocean diagnostics:

- Temperature
- · Salinity
- Nitrate
- Phosphate
- Silicate
- · Dissolved Oxygen

These files need to be reformatted using the esmvaltool data format WOA command.

#### Landschuetzer 2016

These data can be downloaded from: https://www.nodc.noaa.gov/archive/arc0105/0160558/3.3/data/0-data/spco2\_1982-2015\_MPI\_SOM-FFN\_v2016.nc (last access 09/20/2022)

#### The following variables are used by the ocean diagnostics:

- fgco2, Surface Downward Flux of Total CO2
- spco2, Surface Aqueous Partial Pressure of CO2
- dpco2, Delta CO2 Partial Pressure

The file needs to be reformatted using the esmvaltool data format Landschuetzer2016 command.

# 20.6 Sea Surface Salinity Evaluation

#### 20.6.1 Overview

This recipe compares the regional means of sea surface salinity with a reference dataset (ESACCI-SEA-SURFACE-SALINITY v1 or v2 by default). To do this, the recipe generates plots for the timeseries of each region and a radar plot showing (i) the mean state bias, and (ii) the ratio between the simulated and observed standard deviations of different regional averages of sea surface salinity, calculated in the temporal window for which observations and simulations overlap.

#### 20.6.2 Preprocessor requirements:

The recipe is created in a way that should make possible (although is not tested) to use it for other variables and datasets, even for more than one at a time. The diagnostic only expects variables with dimensions *time* and *depth\_id* and it does not assume any other constraint.

It is therefore mandatory to keep the *extract\_shape* preprocessor for more than one region and any form of region operation (*mean, max, min...*) to collapse the *latitude* and *longitude* coordinates. In case you want to try with variables that have extra dimensions (i.e. *depth*) you must add an extra preprocessor call to collapse them (i.e. *depth\_integration*)

The recipe can be used with any shapefile. As it is, it uses the IHO Sea Areas (version 3) downloaded from https: //marineregions.org/downloads.php, but any shapefile containing marine regions can be used.

Any number of regions can be choosed also, even though plots may look odd if too few or too many are selected.

## 20.6.3 Regions available on IHO Sea Areas file:

- Adriatic Sea
- Aegean Sea
- Alboran Sea
- Andaman or Burma Sea
- Arabian Sea
- Arafura Sea
- Arctic Ocean
- Baffin Bay

- Balearic (Iberian Sea)
- Bali Sea
- Baltic Sea
- Banda Sea
- Barentsz Sea
- Bass Strait
- Bay of Bengal
- Bay of Biscay
- Bay of Fundy
- Beaufort Sea
- Bering Sea
- Bismarck Sea
- Black Sea
- Bristol Channel
- Caribbean Sea
- Celebes Sea
- Celtic Sea
- Ceram Sea
- Chukchi Sea
- Coral Sea
- Davis Strait
- East Siberian Sea
- Eastern China Sea
- English Channel
- Flores Sea
- Great Australian Bight
- Greenland Sea
- Gulf of Aden
- Gulf of Alaska
- Gulf of Aqaba
- Gulf of Boni
- Gulf of Bothnia
- Gulf of California
- Gulf of Finland
- Gulf of Guinea
- Gulf of Mexico

- Gulf of Oman
- Gulf of Riga
- Gulf of St. Lawrence
- Gulf of Suez
- Gulf of Thailand
- Gulf of Tomini
- Halmahera Sea
- Hudson Bay
- Hudson Strait
- Indian Ocean
- Inner Seas off the West Coast of Scotland
- Ionian Sea
- Irish Sea and St. George's Channel
- Japan Sea
- Java Sea
- Kara Sea
- Kattegat
- Labrador Sea
- Laccadive Sea
- Laptev Sea
- Ligurian Sea
- Lincoln Sea
- Makassar Strait
- Malacca Strait
- Mediterranean Sea Eastern Basin
- Mediterranean Sea Western Basin
- Molukka Sea
- Mozambique Channel
- North Atlantic Ocean
- North Pacific Ocean
- North Sea
- Norwegian Sea
- Persian Gulf
- Philippine Sea
- Red Sea
- Rio de La Plata

- Savu Sea
- Sea of Azov
- Sea of Marmara
- · Sea of Okhotsk
- Seto Naikai or Inland Sea
- Singapore Strait
- Skagerrak
- Solomon Sea
- South Atlantic Ocean
- South China Sea
- South Pacific Ocean
- Southern Ocean
- Strait of Gibraltar
- Sulu Sea
- Tasman Sea
- The Coastal Waters of Southeast Alaska and British Columbia
- The Northwestern Passages
- Timor Sea
- Tyrrhenian Sea
- White Sea
- Yellow Sea

## 20.6.4 Available recipes and diagnostics

Recipes are stored in recipes/

recipe\_sea\_surface\_salinity.yml

Diagnostics are stored in diag\_scripts/sea\_surface\_salinity/

• compare\_salinity.py: plot timeseries for each region and generate radar plot.

## 20.6.5 User settings in recipe

```
1. compare_salinity.py
```

Required settings for script

none

Optional settings for script

none

Required settings for variables

• ref\_model: name of reference data set

*Optional settings for variables* none

#### 20.6.6 Variables

• sos (ocean, monthly, time latitude longitude)

## 20.6.7 Observations and reformat scripts

• ESACCI-SEA-SURFACE-SALINITY (sos)

## 20.6.8 References

- Diagnostic: please contact authors
- ESACCI-SEA-SURFACE-SALINITY dataset: Boutin, J., J.-L. Vergely, J. Koehler, F. Rouffi, N. Reul: ESA Sea Surface Salinity Climate Change Initiative (Sea\_Surface\_Salinity\_cci): Version 1.8 data collection. Centre for Environmental Data Analysis, 25 November 2019. doi: 10.5285/9ef0ebf847564c2eabe62cac4899ec41. http://dx.doi.org/10.5285/9ef0ebf847564c2eabe62cac4899ec41

## 20.6.9 Example plots

## 20.7 Ocean metrics

## 20.7.1 Overview

The Southern Ocean is central to the global climate and the global carbon cycle, and to the climate's response to increasing levels of atmospheric greenhouse gases. Global coupled climate models and earth system models, however, vary widely in their simulations of the Southern Ocean and its role in, and response to, the ongoing anthropogenic trend. Observationally-based metrics are critical for discerning processes and mechanisms, and for validating and comparing climate and earth system models. New observations and understanding have allowed for progress in the creation of observationally-based data/model metrics for the Southern Ocean.

The metrics presented in this recipe provide a means to assess multiple simulations relative to the best available observations and observational products. Climate models that perform better according to these metrics also better simulate the uptake of heat and carbon by the Southern Ocean. Russell et al. 2018 assessed only a few of the available CMIP5 simulations, but most of the available CMIP5 and CMIP6 climate models can be analyzed with these recipes.

The goal is to create a recipe for recreation of metrics in Russell, J.L., et al., 2018, J. Geophys. Res. – Oceans, 123, 3120-3143, doi: 10.1002/2017JC013461.

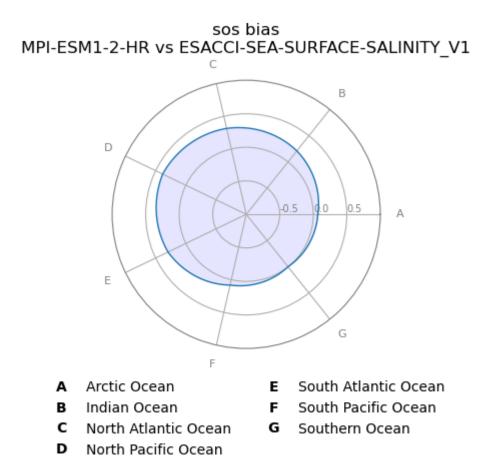


Fig. 11: Radar plot showing the mean state biases (simulation minus observations) for the regional averages of sea surface salinity in the selected ocean basins and seas.

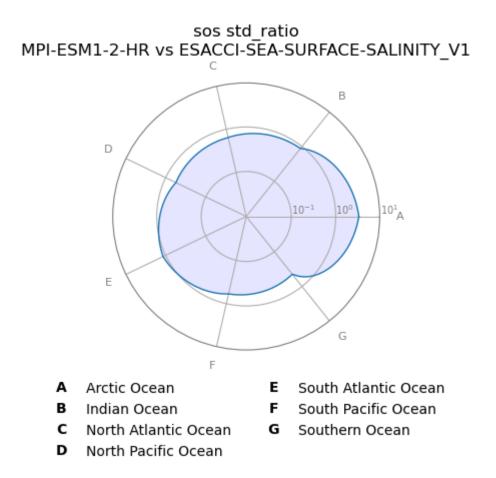


Fig. 12: Radar plot showing the ratio between the simulated and observed standard deviations of the regional averages of sea surface salinity in the selected ocean basins and seas.

#### 20.7.2 Available recipes and diagnostics

Recipes are stored in recipes/

• recipe\_russell18jgr.yml

Diagnostics are stored in diag\_scripts/russell18jgr/

- russell18jgr-polar.ncl (figures 1, 7, 8): calculates and plots annual-mean variables (tauu, sic, fgco2, pH) as polar contour map.
- russell18jgr-fig2.ncl: calculates and plots The zonal and annual means of the zonal wind stress (N/m<sup>2</sup>).
- russell18jgr-fig3b.ncl: calculates and plots the latitudinal position of Subantarctic Front. Using definitions from Orsi et al (1995).
- russell18jgr-fig3b-2.ncl: calculates and plots the latitudinal position of Polar Front. Using definitions from Orsi et al (1995).
- russell18jgr-fig4.ncl: calculates and plots the zonal velocity through Drake Passage (at 69W) and total transport through the passage if the volcello file is available.
- russell18jgr-fig5.ncl: calculates and plots the mean extent of sea ice for September(max) in blue and mean extent of sea ice for February(min) in red.
- russell18jgr-fig5g.ncl: calculates and plots the annual cycle of sea ice area in southern ocean.
- russell18jgr-fig6a.ncl: calculates and plots the density layer based volume transport(in Sv) across 30S based on the layer definitions in Talley (2008).
- russell18jgr-fig6b.ncl: calculates and plots the Density layer based heat transport(in PW) across 30S based on the layer definitions in Talley (2008).
- russell18jgr-fig7h.ncl: calculates and plots the zonal mean flux of fgco2 in gC/(yr \* m<sup>2</sup>).
- russell18jgr-fig7i.ncl: calculates and plots the cumulative integral of the net CO2 flux from 90S to 30S (in PgC/yr).
- russell18jgr-fig9a.ncl: calculates and plots the scatter plot of the width of the Southern Hemisphere westerly wind band against the annual-mean integrated heat uptake south of 30S (in PW), along with the line of best fit.
- russell18jgr-fig9b.ncl: calculates and plots the scatter plot of the width of the Southern Hemisphere westerly wind band against the annual-mean integrated carbon uptake south of 30S (in Pg C/yr), along with the line of best fit.
- russell18jgr-fig9c.ncl: calculates and plots the scatter plot of the net heat uptake south of 30S (in PW) against the annual-mean integrated carbon uptake south of 30S (in Pg C/yr), along with the line of best fit.

## 20.7.3 User settings in recipe

1. Script russell18jgr-polar.ncl

Required settings (scripts)

- styleset : CMIP5(recommended), default, etc.
- ncdf : default(recommended), CMIP5, etc.
- max\_lat : -30.0

Optional settings (scripts)

• grid\_max : 0.4 (figure 1), 30 (figure 7), 8.2 (figure 8)

- grid\_min : -0.4 (figure 1), -30 (figure 7), 8.0 (figure 8)
- grid\_step : 0.1 (figure 1), 2.5 (figure 7), 0.1 (figure 8)
- colormap : BlWhRe (figure 7)
- colors: [[237.6, 237.6, 0.], [255, 255, 66.4], [255, 255, 119.6], [255, 255, 191.8], [223.8, 191.8, 223.8], [192.8, 127.5, 190.8], [161.6, 65.3, 158.6], [129.5, 1.0, 126.5] ] (figure 1) [[132,12,127], [147,5,153], [172,12,173], [195,33,196], [203,63,209], [215,89,225], [229,117,230], [243,129,238], [253,155,247], [255,178,254], [255,255,255], [125,255,255], [126,240,138], [134,234,138], [95,219,89], [57,201,54], [39,182,57], [33,161,36], [16,139,22], [0,123,10], [6,96,6], [12,77,9.0] ] (figure 8)
- max\_vert : 1 4 (user preference)
- max\_hori : 1 4 (user preference)
- grid\_color: blue4 (figure 8)
- labelBar\_end\_type: ExcludeOuterBoxes (figure 1), both\_triangle (figure 7, 8)
- unitCorrectionalFactor: -3.154e+10 (figure 7)
- new\_units : "gC/ (m~S~2~N~ \* yr)" (figure 7)

Required settings (variables)

• additional\_dataset: datasets to plot.

Optional settings (variables)

- none
- 2. Script russell18jgr-fig2.ncl

Required settings (scripts)

- styleset : CMIP5(recommended), default, etc.
- ncdf : default(recommended), CMIP5, etc.

Optional settings (scripts)

- none
- 3. Script russell18jgr-fig3b.ncl

Required settings (scripts)

- styleset : CMIP5(recommended), default, etc.
- ncdf : default(recommended), CMIP5, etc.

Optional settings (scripts)

• none

4. Script russell18jgr-fig3b-2.ncl

Required settings (scripts)

- styleset : CMIP5(recommended), default, etc.
- ncdf : default(recommended), CMIP5, etc.

Optional settings (scripts)

• none

- 5. Script russell18jgr-fig4.ncl
  - Required settings (scripts)
    - styleset : CMIP5(recommended), default, etc.
    - ncdf : default(recommended), CMIP5, etc.

Optional settings (scripts)

- max\_vert : 1 4 (user preference)
- max\_hori : 1 4 (user preference)
- unitCorrectionalFactor: 100 (m/s to cm/s)
- new\_units : "cm/s"
- 6. Script russell18jgr-fig5.ncl

#### Required settings (scripts)

- styleset : CMIP5(recommended), default, etc.
- ncdf : default(recommended), CMIP5, etc.
- max\_lat : -45.0

Optional settings (scripts)

- max\_vert : 1 4 (user preference)
- max\_hori : 1 4 (user preference)
- 7. Script russell18jgr-fig5g.ncl

Required settings (scripts)

• styleset : CMIP5(recommended), default, etc.

Optional settings (scripts)

- none
- 8. Script russell18jgr-fig6a.ncl

#### Required settings (scripts)

- styleset : CMIP5(recommended), default, etc.
- ncdf : default(recommended), CMIP5, etc.

Optional settings (scripts)

• none

9. Script russell18jgr-fig6b.ncl

#### Required settings (scripts)

- styleset : CMIP5(recommended), default, etc.
- ncdf : default(recommended), CMIP5, etc.

Optional settings (scripts)

• none

10. Script russell18jgr-fig7h.ncl

Required settings (scripts)

- styleset : CMIP5(recommended), default, etc.
- ncdf : default(recommended), CMIP5, etc.

Optional settings (scripts)

- none
- 11. Script russell18jgr-fig7i.ncl
  - Required settings (scripts)
    - styleset : CMIP5(recommended), default, etc.
    - ncdf : default(recommended), CMIP5, etc.

Optional settings (scripts)

- none
- 12. Script russell18jgr-fig9a.ncl

Required settings (scripts)

- styleset : CMIP5(recommended), default, etc.
- ncdf : default(recommended), CMIP5, etc.

Optional settings (scripts)

- none
- 13. Script russell18jgr-fig9b.ncl

Required settings (scripts)

- styleset : CMIP5(recommended), default, etc.
- ncdf : default(recommended), CMIP5, etc.

Optional settings (scripts)

- none
- 14. Script russell18jgr-fig9c.ncl

Required settings (scripts)

- styleset : CMIP5(recommended), default, etc.
- ncdf : default(recommended), CMIP5, etc.

Optional settings (scripts)

• none

## 20.7.4 Variables

- tauu (atmos, monthly mean, longitude latitude time)
- tauuo, hfds, fgco2 (ocean, monthly mean, longitude latitude time)
- thetao, so, vo (ocean, monthly mean, longitude latitude lev time)
- pH (ocnBgchem, monthly mean, longitude latitude time)
- uo (ocean, monthly mean, longitude latitude lev time)
- sic (seaIce, monthly mean, longitude latitude time)

## 20.7.5 Observations and reformat scripts

#### Note: WOA data has not been tested with reciepe\_russell18jgr.yml and

corresponding diagnostic scripts.

• WOA (thetao, so - esmvaltool/cmorizers/data/formatters/datasets/woa.py)

## 20.7.6 References

- Russell, J.L., et al., 2018, J. Geophys. Res. Oceans, 123, 3120-3143. https://doi.org/10.1002/2017JC013461
- Talley, L.D., 2003. Shallow,intermediate and deep overturning components of the global heat budget. Journal of Physical Oceanography 33, 530–560

## 20.7.7 Example plots

#### CanESM2

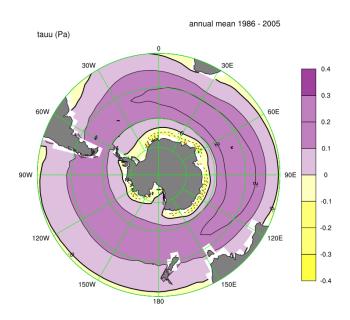


Fig. 13: Figure 1: Annual-mean zonal wind stress (tauu -  $N/m^2$ ) with eastward wind stress as positive plotted as a polar contour map.

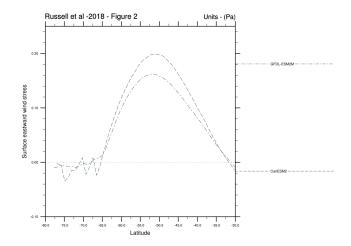


Fig. 14: Figure 2: The zonal and annual means of the zonal wind stress (N/m<sup>2</sup>) plotted in a line plot.

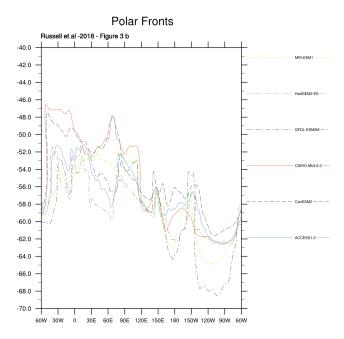


Fig. 15: Figure 3a: The latitudinal position of Subantarctic Front using definitions from Orsi et al (1995).

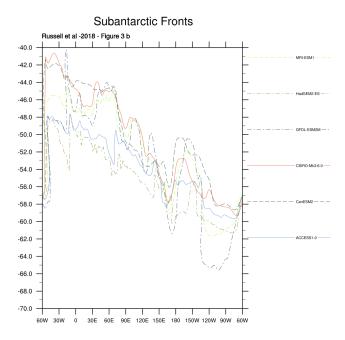


Fig. 16: Figure 3b: The latitudinal position of Polar Front using definitions from Orsi et al (1995).

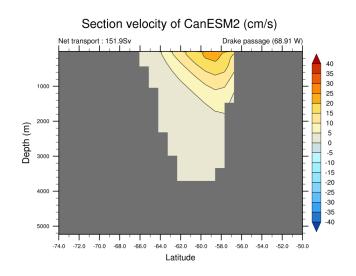


Fig. 17: Figure 4: Time averaged zonal velocity through Drake Passage (at 69W, in cm/s, eastward is positive). The total transport by the ACC is calculated if volcello file is available.

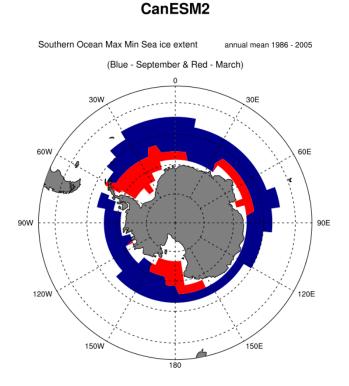


Fig. 18: Figure 5: Mean extent of sea ice for September(max) in blue and February(min) in red plotted as polar contour map.

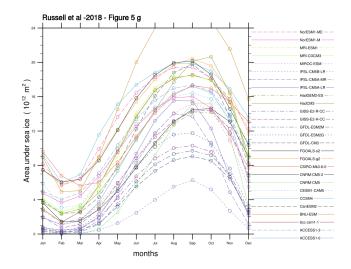


Fig. 19: Figure 5g: Annual cycle of sea ice area in southern ocean as a line plot (monthly climatology).

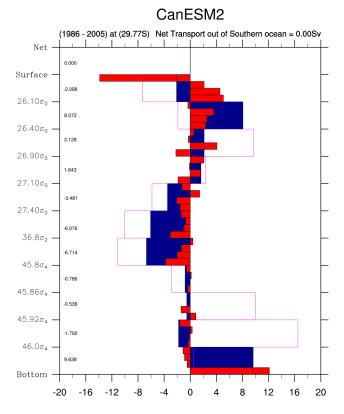


Fig. 20: Figure 6a: Density layer based volume transport (in Sv) across 30S based on the layer definitions in Talley (2008).

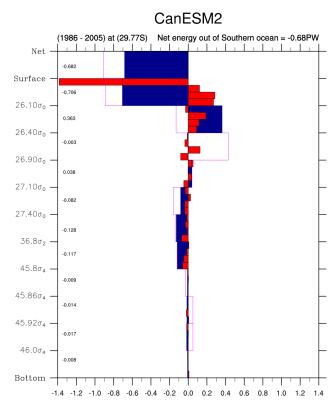


Fig. 21: Figure 6b: Density layer based heat transport(in PW) across 30S based on the layer definitions in Talley (2008).

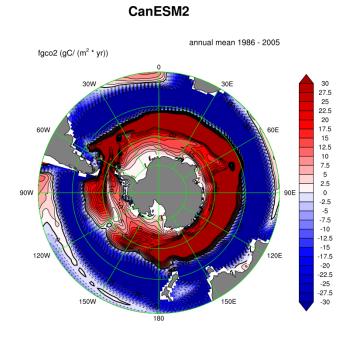


Fig. 22: Figure 7: Annual mean  $CO_2$  flux (sea to air,  $gC/(yr * m^2)$ , positive (red) is out of the ocean) as a polar contour map.

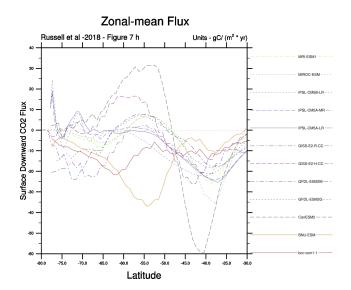


Fig. 23: Figure 7h: the time and zonal mean flux of  $CO_2$  in  $gC/(yr * m^2)$  plotted as a line plot.

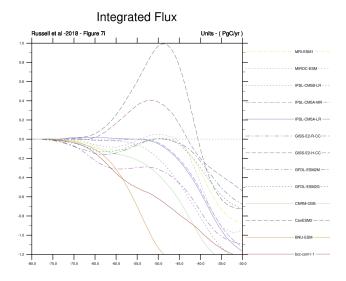
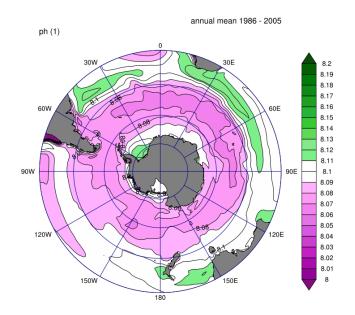


Fig. 24: Figure 7i is the cumulative integral of the net CO<sub>2</sub> flux from 90S to 30S (in PgC/yr) plotted as a line plot.



#### MRI-ESM1

Fig. 25: Figure 8: Annual-mean surface pH plotted as a polar contour map.

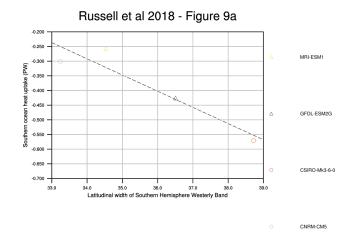


Fig. 26: Figure 9a: Scatter plot of the width of the Southern Hemisphere westerly wind band (in degrees of latitude) against the annual-mean integrated heat uptake south of 30S (in PW—negative uptake is heat lost from the ocean) along with the best fit line.

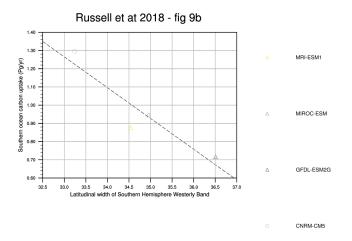
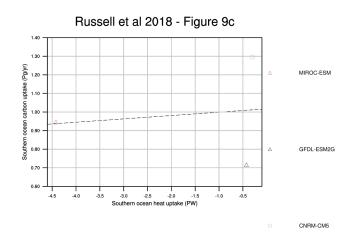
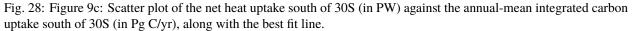


Fig. 27: Figure 9b: Scatter plot of the width of the Southern Hemisphere westerly wind band (in degrees of latitude) against the annual-mean integrated carbon uptake south of 30S (in Pg C/yr), along with the best fit line.





## CHAPTER

## TWENTYONE

## OTHER

# 21.1 Capacity factor of wind power: Ratio of average estimated power to theoretical maximum power

#### 21.1.1 Overview

The goal of this diagnostic is to compute the wind capacity factor, taking as input the daily instantaneous surface wind speed, which is then extrapolated to obtain the wind speed at a height of 100 m as described in Lledó (2017).

The capacity factor is a normalized indicator of the suitability of wind speed conditions to produce electricity, irrespective of the size and number of installed turbines. This indicator is provided for three different classes of wind turbines (IEC, 2005) that are designed specifically for low, medium and high wind speed conditions.

The user can select the region, temporal range and season of interest.

The output of the recipe is a netcdf file containing the capacity factor for each of the three turbine classes.

#### 21.1.2 Available recipes and diagnostics

Recipes are stored in recipes/

recipe\_capacity\_factor.yml

Diagnostics are stored in diag\_scripts/magic\_bsc/

- capacity\_factor.R: calculates the capacity factor for the three turbine classes.
- PC.R: calculates the power curves for the three turbine classes.

## 21.1.3 User settings

User setting files are stored in recipes/

1. recipe\_capacity\_factor.yml

Required settings for script

• power\_curves: (should not be changed)

#### 21.1.4 Variables

• sfcWind (atmos, daily, longitude, latitude, time)

## 21.1.5 Observations and reformat scripts

Main features of the selected turbines:

Turbine na	me	Rotor (m)	diameter	Rated (MW)	power	Cut-in (m/s)	speed	Rated (m/s)	speed	Cut-out (m/s)	speed
Enercon 2.3MW	E70	70		2.3		2.0		16.0		25.0	
Gamesa 2.0MW	G80	80		2.0		4.0		17.0		25.0	
Gamesa 2.0MW	G87	87		2.0		4.0		16.0		25.0	
Vestas 2.0MW	V100	100		2.0		3.0		15.0		20.0	
Vestas 2.0MW	V110	110		2.0		3.0		11.5		20.0	

## 21.1.6 References

- IEC. (2005). International Standard IEC 61400-1, third edition, International Electrotechnical Commission. https://webstore.iec.ch/preview/info\_iec61400-1%7Bed3.0%7Den.pdf
- Lledó, L. (2017). Computing capacity factor. Technical note BSC-ESS-2017-001, Barcelona Supercomputing Center. Available online at https://earth.bsc.es/wiki/lib/exe/fetch.php?media=library:external: bsc-ess-2017-001-c4e\_capacity\_factor.pdf [last accessed 11 October 2018]

## 21.1.7 Example plots

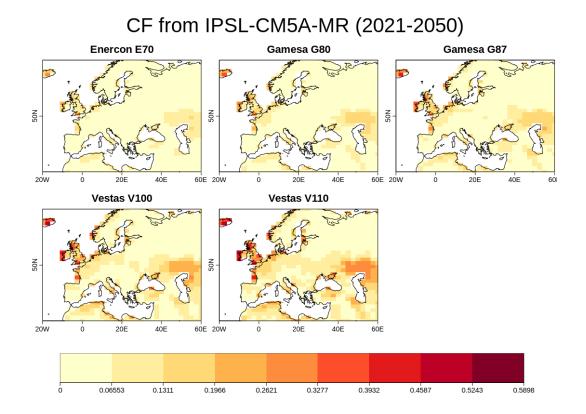
Wind capacity factor for five turbines: Enercon E70 (top-left), Gamesa G80 (middle-top), Gamesa G87 (top-right), Vestas V100 (bottom-left) and Vestas V110 (middle-bottom) using the IPSL-CM5A-MR simulations for the r1p1i1 ensemble for the rcp8.5 scenario during the period 2021-2050.

# 21.2 CMORizer recipes

## 21.2.1 Overview

These are CMORizer recipes calling CMORizer diagnostic scripts.

ESMValCore supports ERA5 hourly and monthly datasets in their native format, see *Datasets in native format*. and ERA5 data documentation. It may be useful in some cases to create ERA5 daily CMORized data. This can be achieved by using a CMORizer *recipe*, see recipe\_daily\_era5.yml. This recipe reads native, hourly ERA5 data, performs a daily aggregation preprocessor, and then calls a diagnostic that operates on the data. In this example, the diagnostic renames the files to the standard OBS6 file names. The output are thus daily, CMORized ERA5 data, that can be used through the OBS6 project. As such, this example recipe creates a local pool of CMORized data. The advantage, in this case, is that the daily aggregation is performed only once, which can save a lot of time and compute if it is used often.



The example CMORizer recipe can be run like any other ESMValTool recipe:

```
esmvaltool run cmorizers/recipe_daily_era5.yml
```

Note that the recipe\_daily\_era5.yml adds the next day of the new year to the input data. This is because one of the fixes needed for the ERA5 data is to shift the time axis of non-instantaneous variables half an hour back in time, resulting in a missing record on the last day of the year. ERA5 data can be downloaded using era5cli.

## 21.2.2 Available recipes and diagnostics

Recipes are stored in esmvaltool/recipes/

• cmorizers/recipe\_daily\_era5.yml

Diagnostics are stored in esmvaltool/diag\_scripts/

• cmorizers/era5.py: generates output filename

## 21.2.3 User settings in recipe

1. cmorizers/recipe\_daily\_era5.yml

Required add\_one\_day preprocessor settings:

- start\_year: 1990
- start\_month: 1
- start\_day: 1
- end\_year: 1991

- end\_month: 1
- end\_day: 1

#### These settings should not be changed

• daily\_mean:

operator: mean

- daily\_min: operator: min
- daily\_max:
  - operator: max

#### 21.2.4 Variables

- 1. cmorizers/recipe\_daily\_era5.yml
  - clt
  - evspsbl
  - evspsblpot
  - mrro
  - pr
  - prsn
  - ps
  - psl
  - rlds
  - rls
  - rsds
  - rsdt
  - rss
  - tas
  - tasmax
  - tasmin
  - tdps
  - ts
  - tsn
  - uas
  - vas

#### 21.2.5 References

• Hersbach, H., et al., Quarterly Journal of the Royal Meteorological Society, 730, 1999-2049, doi:10.1002/qj.3803, 2020.

# 21.3 Ensemble Clustering - a cluster analysis tool for climate model simulations (EnsClus)

#### 21.3.1 Overview

EnsClus is a cluster analysis tool in Python, based on the k-means algorithm, for ensembles of climate model simulations.

Multi-model studies allow to investigate climate processes beyond the limitations of individual models by means of inter-comparison or averages of several members of an ensemble. With large ensembles, it is often an advantage to be able to group members according to similar characteristics and to select the most representative member for each cluster.

The user chooses which feature of the data is used to group the ensemble members by clustering: time mean, maximum, a certain percentile (e.g., 75% as in the examples below), standard deviation and trend over the time period. For each ensemble member this value is computed at each grid point, obtaining N lat-lon maps, where N is the number of ensemble members. The anomaly is computed subtracting the ensemble mean of these maps to each of the single maps. The anomaly is therefore computed with respect to the ensemble members (and not with respect to the time) and the Empirical Orthogonal Function (EOF) analysis is applied to these anomaly maps.

Regarding the EOF analysis, the user can choose either how many Principal Components (PCs) to retain or the percentage of explained variance to keep. After reducing dimensionality via EOF analysis, k-means analysis is applied using the desired subset of PCs.

The major final outputs are the classification in clusters, i.e. which member belongs to which cluster (in k-means analysis the number k of clusters needs to be defined prior to the analysis) and the most representative member for each cluster, which is the closest member to the cluster centroid.

Other outputs refer to the statistics of clustering: in the PC space, the minimum and the maximum distance between a member in a cluster and the cluster centroid (i.e. the closest and the furthest member), the intra-cluster standard deviation for each cluster (i.e. how much the cluster is compact).

#### 21.3.2 Available recipes and diagnostics

Recipes are stored in recipes/

• recipe\_ensclus.yml

Diagnostics are stored in diag\_scripts/ensclus/

ensclus.py

and subroutines

- ens\_anom.py
- ens\_eof\_kmeans.py
- ens\_plots.py
- eof\_tool.py
- read\_netcdf.py

• sel\_season\_area.py

## 21.3.3 User settings

Required settings for script

- season: season over which to perform seasonal averaging (DJF, DJFM, NDJFM, JJA)
- area: region of interest (EAT=Euro-Atlantic, PNA=Pacific North American, NH=Northern Hemisphere, EU=Europe)
- extreme: extreme to consider: XXth\_percentile (XX can be set arbitrarily, e.g. 75th\_percentile), mean (mean value over the period), maximum (maximum value over the period), std (standard deviation), trend (linear trend over the period)
- numclus: number of clusters to be computed
- perc: percentage of variance to be explained by PCs (select either this or numpcs, default=80)
- numpes: number of PCs to retain (has priority over perc unless it is set to 0 (default))

#### Optional settings for script

• max\_plot\_panels: maximum number of panels (datasets) in a plot. When exceeded multiple plots are created. Default: 72

## 21.3.4 Variables

• chosen by user (e.g., precipitation as in the example)

## 21.3.5 Observations and reformat scripts

None.

## 21.3.6 References

 Straus, D. M., S. Corti, and F. Molteni: Circulation regimes: Chaotic variability vs. SST forced predictability. J. Climate, 20, 2251–2272, 2007. https://doi.org/10.1175/JCLI4070.1

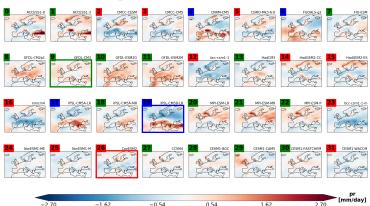
## 21.3.7 Example plots

# 21.4 ESA CCI LST comparison to Historical Models

## 21.4.1 Overview

This diagnostic compares ESA CCI LST to multiple historical emsemble members of CMIP models. It does this over a defined region for monthly values of the land surface temperature. The result is a plot showing the mean differnce of CCI LST to model average LST, with a region of +/- one standard deviation of the model mean LST given as a measure of model variability.

The recipe and diagnostic need the all time average monthly LST from the CCI data. We use the L3C single sensor monthy data. A CMORizing script calculates the mean of the day time, and night time overpasses to give the all time



Anomalies pr 75th\_percentile EU JJA CMIP5 historical 1900-2005

Fig. 1: Clustering based on the 75th percentile of historical summer (JJA) precipitation rate for CMIP5 models over 1900-2005. 3 clusters are computed, based on the principal components explaining 80% of the variance. The 32 models are grouped in three different clusters. The green cluster is the most populated with 16 ensemble members mostly characterized by a positive anomaly over central-north Europe. The red cluster counts 12 elements that exhibit a negative anomaly centered over southern Europe. The third cluster – labelled in blue- includes only 4 models showing a north-south dipolar precipitation anomaly, with a wetter than average Mediterranean counteracting dryer North-Europe. Ensemble members No.9, No.26 and No.19 are the "specimen" of each cluster, i.e. the model simulations that better represent the main features of that cluster. These ensemble members can eventually be used as representative of the whole possible outcomes of the multi-model ensemble distribution associated to the 32 CMIP5 historical integrations for the summer precipitation rate 75 th percentile over Europe when these outcomes are reduced from 32 to 3. The number of ensemble members of each cluster might provide a measure of the probability of occurrence of each cluster.

average LST. This is so that the Amon output from CMIP models can be used. We created such a dataset from the Aqua MODIS data from CCI.

#### 21.4.2 Available recipes and diagnostics

Recipes are stored in esmvaltool/recipes/

recipe\_esacci\_lst.yml

Diagnostics are stored in esmvaltool/diag\_scripts/lst/

• lst.py

#### 21.4.3 User settings in recipe

- Script recipe\_esacci\_lst.yml
  - No required settings for script

No user defined inputs to the diagnostic

Required settings for variables

• The diagnostic works with all data sources on having the same start\_year and end\_year, and hence that data is also available.

Required settings for preprocessor

• start\_longitude, end\_longitude The western and eastern bounds of the region to work with.

- start\_latitude, end\_latitude The southern and northern bounds of the region to work with.
- target\_grid This should be one of the model grids.

#### 21.4.4 Variables

• ts (atmos, monthly mean, longitude latitude time)

#### 21.4.5 Observations and reformat scripts

This recipe and diagnostic is written to work with data created from the CMORizer esmvaltool/cmorizers/obs/cmorize\_obs\_esacci\_lst.py. This takes the orginal ESA CCI LST files for the L3C data from Aqua MODIS DAY and NIGHT files and creates a the all time mean data this diagnostic uses. Advice from the CCI LST team is to use the monthly not daily files to create the all time average to avoid the possibility of biasing towards night time LST values being more prevalent because of how the cloud screening algorithms work.

#### 21.4.6 References

• ESA CCI LST project https://climate.esa.int/en/projects/land-surface-temperature/

#### 21.4.7 Example plots

### **21.5 Timeseries for Arctic-Midlatitude Teleconnections**

#### 21.5.1 Overview

The recipe produces the timeseries of selected variables to study Arctic-midlatitude teleconnections for further application of Causal Model Evaluation (CME) described in Galytska et al. (2023).

The output of the recipe consists of the .nc files named after the data source (e.g. ERA5, ACCESS-CM2.nc etc.). Each file contains the area-weighted spatial average of climatological monthly anomalies of selected variables. The recipe also applies the CVDP package.

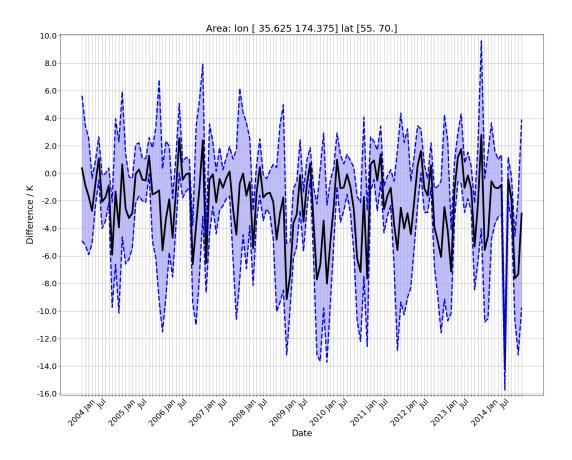
#### 21.5.2 Available recipes and diagnostics

Recipes are stored in esmvaltool/recipes/

• recipe\_galytska23jgr.yml

Diagnostics are stored in esmvaltool/diag\_scripts/

- galytska23/select\_variables\_for\_tigramite.py
- cvdp/cvdp\_wrapper.py



#### ESACCI LST - CMIP6 Historical Ensemble Mean

Fig. 2: Timeseries of the ESA CCI LST minus mean of CMIP6 ensembles. The selected region is 35E-175E, 55N-70N. The black line is the mean difference, and the blue shaded area denotes one standard deviation either way of the individual ensemble member's difference in LST. Models used for this are UKESM1 members r1i1p1f2 and r2i1p1f2, and CESM members r2i1p1f1 and r3i1p1f1. We have used the entire timeseries of available CCI data 2004-2014 inclusive, noting we have not written the CMORizer to process the incomplete year of 2003 for the Aqua MODIS data.

#### 21.5.3 User settings in recipe

- 1. Preprocessor
  - anomalies (period: monthly): Calculate anomalies for selected variables
  - regrid (target\_grid: 1x1): Linear regridding of all datasets to the uniform grid
  - area\_statistics (operation: mean): Calculate mean over defined regions
- 2. Script <select\_variables\_for\_tigramite.py>

none

3. Script <cvdp\_wrapper.py>

none

- 4. Script <cvdp/cvdp/driver.ncl>
  - modular (modular: True): Run the diagnostics that is selected in modular\_list
  - modular\_list (modular\_list: psl.nam\_nao): Calculate only NAO diagnostics

#### 21.5.4 Variables

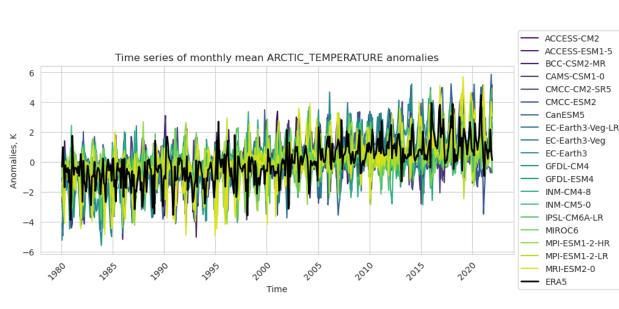
- zg (atmos, monthly mean, longitude latitude time)
- tas (atmos, monthly mean, longitude latitude time)
- psl (atmos, monthly mean, longitude latitude time)
- va (atmos, monthly mean, longitude latitude time)
- ta (atmos, monthly mean, longitude latitude time)
- sic/siconc (seaice, monthly mean, longitude latitude time)
- ts (atmos, monthly mean, longitude latitude time)
- pr (atmos, monthly mean, longitude latitude time)

#### 21.5.5 Observations and reformat scripts

- ERA5 (pr, psl, ta, tas, ts, va, zg ERA5 data can be used via the native6 project)
- HadISST (sic esmvaltool/cmorizers/data/formatters/datasets/hadisst.ncl)

#### 21.5.6 References

- Galytska, E., Weigel, K., Handorf, D., Jaiser, R., Köhler, R. H., Runge, J., & Eyring, V.: Causal model evaluation of Arctic-midlatitude teleconnections in CMIP6. Authorea Preprints. https://doi.org/10.1002/essoar.10512569. 1.
- Copernicus Climate Change Service (C3S), 2017: ERA5: Fifth generation of ECMWF atmospheric reanalyses of the global climate, edited, Copernicus Climate Change Service Climate Data Store (CDS). https://cds.climate.copernicus.eu/cdsapp#!/home
- http://www.cesm.ucar.edu/working\_groups/CVC/cvdp/



#### 21.5.7 Example plots

Fig. 3: Monthly mean temperature anomalies in the Arctic  $(65^{\circ}-90^{\circ}N)$  from observations and selected CMIP6 models during 1980-2021.

## 21.6 Multi-model products

#### 21.6.1 Overview

The goal of this diagnostic is to compute the multi-model ensemble mean for a set of models selected by the user for individual variables and different temporal resolutions (annual, seasonal, monthly).

After selecting the region (defined by the lowermost and uppermost longitudes and latitudes), the mean for the selected reference period is subtracted from the projections in order to obtain the anomalies for the desired period. In addition, the recipe computes the percentage of models agreeing on the sign of this anomaly, thus providing some indication on the robustness of the climate signal.

The output of the recipe consists of a colored map showing the time average of the multi-model mean anomaly and stippling to indicate locations where the percentage of models agreeing on the sign of the anomaly exceeds a threshold selected by the user. Furthermore, a time series of the area-weighted mean anomaly for the projections is plotted. For the plots, the user can select the length of the running window for temporal smoothing and choose to display the ensemble mean with a light shading to represent the spread of the ensemble or choose to display each individual models.

#### 21.6.2 Available recipes and diagnostics

Recipes are stored in recipes/

• recipe\_multimodel\_products.yml

Diagnostics are stored in diag\_scripts/magic\_bsc/

• multimodel\_products.R - script for computing multimodel anomalies and their agreement.

#### 21.6.3 User settings

User setting files are stored in recipes/

1. recipe\_multimodel\_products.yml

Required settings for script

- colorbar\_lim: positive number specifying the range (-colorbar\_lim ... +colorbar\_lim) of the colorbar (0 = automatic colorbar scaling)
- moninf: integer specifying the first month of the seasonal mean period to be computed
- monsup: integer specifying the last month of the seasonal mean period to be computed, if it's null the anomaly of month indicated in moninf will be computed
- agreement\_threshold: integer between 0 and 100 indicating the threshold in percent for the minimum agreement between models on the sign of the multi-model mean anomaly for the stipling to be plotted
- running\_mean: integer indictating the length of the window for the running mean to be computed
- time\_series\_plot: Either single or maxmin (plot the individual or the mean with shading between the max and min).

#### 21.6.4 Variables

• any Amon variable (atmos, monthly mean, longitude latitude time)

#### 21.6.5 Observations and reformat scripts

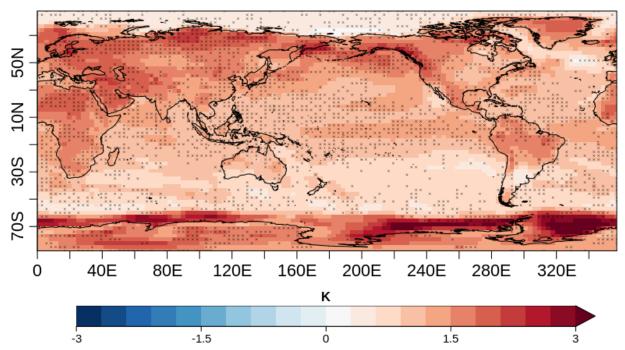
None

#### 21.6.6 References

- Hagedorn, R., Doblas-Reyes, F. J., Palmer, T. N., Nat E H Ag E D O R N, R. E., & Pa, T. N. (2005). The rationale behind the success of multi-model ensembles in seasonal forecasting-I. Basic concept, 57, 219–233. https://doi.org/10.3402/tellusa.v57i3.14657
- Weigel, A. P., Liniger, M. A., & Appenzeller, C. (2008). Can multi-model combination really enhance the prediction skill of probabilistic ensemble forecasts? Quarterly Journal of the Royal Meteorological Society, 134(630), 241–260. https://doi.org/10.1002/qj.210

#### 21.6.7 Example plots

Multi-model mean anomaly of 2-m air temperature during the future projection 2006-2099 in June considering the reference period 1961-1990 (colours). Crosses indicate that the 80% of models agree in the sign of the multi-model mean anomaly. The models selected are BCC-CSM1-1, MPI-ESM-MR and MIROC5 in the r1i1p1 ensembles for the RCP 2.6 scenario.



## JUN tas anomaly (2006-2099) - (1961-1990)

## 21.7 Capacity factor for solar photovoltaic (PV) systems

#### 21.7.1 Overview

This diagnostic computes the photovoltaic (PV) capacity factor, a measure of the fraction of the maximum possible energy produced per PV grid cell. It uses the daily incoming surface solar radiation and the surface temperature with a method described in Bett and Thornton (2016). The user can select temporal range, season, and region of interest.

#### 21.7.2 Available recipes and diagnostics

Recipes are stored in recipes/

recipe\_pv\_capacity\_factor.yml

Diagnostics are stored in diag\_scripts/pv\_capacityfactor/

- pv\_capacity\_factor.R: prepares data and plots results.
- PV\_CF.R: calculates the daily capacity factor.

#### 21.7.3 User settings

User setting files are stored in recipes/

1. recipe\_capacity\_factor.yml

Required settings for script

• season: String to include shortcut for season in plot title and name (e.g. "djf"). It will be converted to upper case. This season should be the one set in the preprocessor, since it is only used as a string and does not affect the data in the diagnostic. In the default recipe this is solved through a node anchor.

Optional settings for script

• maxval\_colorbar: Optional upper limit for the colorbar.

#### 21.7.4 Variables

- tas (atmos, daily, longitude, latitude, time)
- rsds (atmos, daily, longitude, latitude, time)

#### 21.7.5 Observations and reformat scripts

• ERA-Interim

#### 21.7.6 References

• Bett, P. E. and Thornton, H. E.: The climatological relationships between wind and solar energy supply in Britain, Renew. Energ., 87, 96–110, https://doi.org/10.1016/j.renene.2015.10.006, 2016.

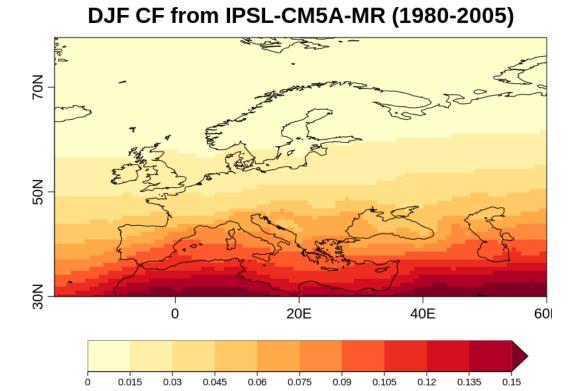
#### 21.7.7 Example plots

PV capacity factor calculated from IPSL-CM5-MR during the DJF season for 1980–2005.

## 21.8 RainFARM stochastic downscaling

#### 21.8.1 Overview

Precipitation extremes and small-scale variability are essential drivers in many climate change impact studies. However, the spatial resolution currently achieved by global and regional climate models is still insufficient to correctly identify the fine structure of precipitation intensity fields. In the absence of a proper physically based representation, this scale gap can be at least temporarily bridged by adopting a stochastic rainfall downscaling technique (Rebora et al, 2006). With this aim, the Rainfall Filtered Autoregressive Model (RainFARM) was developed to apply the stochastic precipitation downscaling method to climate models. The RainFARM Julia library and command-line tool version (https://github.com/jhardenberg/RainFARM.jl) was implemented as recipe. The stochastic method allows to predict climate variables at local scale from information simulated by climate models at regional scale: It first evaluates the statistical distribution of precipitation fields at regional scale and then applies the relationship to the boundary conditions of the climate model to produce synthetic fields at the requested higher resolution. RainFARM exploits the nonlinear transformation of a Gaussian random precipitation field, conserving the information present in the fields at larger scale (Rebora et al., 2006; D'Onofrio et al., 2014).



## 21.8.2 Available recipes and diagnostics

Recipes are stored in recipes/

• recipe\_rainfarm.yml

Diagnostics are stored in diag\_scripts/rainfarm/

• rainfarm.jl

#### 21.8.3 User settings

Required settings for script

- slope: spatial spectral slope (set to 0 to compute automatically from large scales)
- nens: number of ensemble members to be calculated
- nf: number of subdivisions for downscaling (e.g. 8 will produce output fields with linear resolution increased by a factor 8)
- conserv\_glob: logical, if to conserve precipitation over full domain
- conserv\_smooth: logical, if to conserve precipitation using convolution (if neither conserv\_glob or conserv\_smooth is chosen, box conservation is used)
- weights\_climo: set to false or omit if no orographic weights are to be used, else set it to the path to a fine-scale precipitation climatology file. If a relative file path is used, *auxiliary\_data\_dir* will be searched for this file. The file is expected to be in NetCDF format and should contain at least one precipitation field. If several fields at different times are provided, a climatology is derived by time averaging. Suitable climatology files could be for example a fine-scale precipitation climatology from a high-resolution regional climate model (see e.g. Terzago et

al. 2018), a local high-resolution gridded climatology from observations, or a reconstruction such as those which can be downloaded from the WORLDCLIM (http://www.worldclim.org) or CHELSA (http://chelsa-climate.org) websites. The latter data will need to be converted to NetCDF format before being used (see for example the GDAL tools (https://www.gdal.org).

#### 21.8.4 Variables

• pr (atmos, daily mean, longitude latitude time)

#### 21.8.5 Observations and reformat scripts

None.

#### 21.8.6 References

- Terzago et al. 2018, Nat. Hazards Earth Syst. Sci., 18, 2825-2840
- D'Onofrio et al. 2014, J of Hydrometeorology 15, 830-843
- Rebora et. al 2006, JHM 7, 724

#### 21.8.7 Example plots

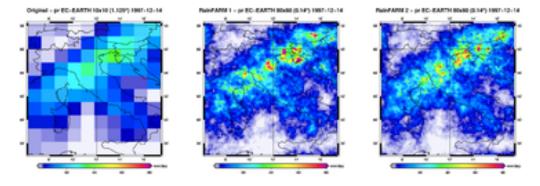


Fig. 4: Example of daily cumulated precipitation from the CMIP5 EC-EARTH model on a specific day, downscaled using RainFARM from its original resolution  $(1.125^{\circ})$  (left panel), increasing spatial resolution by a factor of 8 to  $0.14^{\circ}$ ; Two stochastic realizations are shown (central and right panel). A fixed spectral slope of s=1.7 was used. Notice how the downscaled fields introduce fine scale precipitation structures, while still maintaining on average the original coarse-resolution precipitation. Different stochastic realizations are shown to demonstrate how an ensemble of realizations can be used to reproduce unresolved subgrid variability. (N.B.: this plot was not produced by ESMValTool - the recipe output is netcdf only).

#### 21.9 Sea Ice

#### 21.9.1 Overview

The sea ice diagnostics include:

- (1) time series of Arctic and Antarctic sea ice area and extent (calculated as the total area (km<sup>2</sup>) of grid cells with sea ice concentrations (sic) of at least 15%).
- (2) ice extent trend distributions for the Arctic in September and the Antarctic in February.
- (3) calculation of year of near disappearance of Arctic sea ice
- (4) scatter plots of (a) historical trend in September Arctic sea ice extent (SSIE) vs historical long-term mean SSIE;(b) historical SSIE mean vs 1st year of disappearance (YOD) RCP8.5; (c) historical SSIE trend vs YOD RCP8.5.

#### 21.9.2 Available recipes and diagnostics

Recipes are stored in recipes/

• recipe\_seaice.yml

Diagnostics are stored in diag\_scripts/seaice/

- seaice\_aux.ncl: contains functions for calculating sea ice area or extent from sea ice concentration and first year of disappearance
- seaice\_ecs.ncl: scatter plots of mean/trend of historical September Arctic sea ice extent vs 1st year of disappearance (RCP8.5) (similar to IPCC AR5 Chapter 12, Fig. 12.31a)
- seaice\_trends.ncl: calculates ice extent trend distributions (similar to IPCC AR5 Chapter 9, Fig. 9.24c/d)
- seaice\_tsline.ncl: creates a time series line plots of total sea ice area and extent (accumulated) for northern and southern hemispheres with optional multi-model mean and standard deviation. One value is used per model per year, either annual mean or the mean value of a selected month (similar to IPCC AR5 Chapter 9, Fig. 9.24a/b)
- seaice\_yod.ncl: calculation of year of near disappearance of Arctic sea ice

#### 21.9.3 User settings in recipe

1. Script seaice\_ecs.ncl

Required settings (scripts)

- hist\_exp: name of historical experiment (string)
- month: selected month (1, 2, ..., 12) or annual mean ("A")
- rcp\_exp: name of RCP experiment (string)
- region: region to be analyzed ( "Arctic" or "Antarctic")

Optional settings (scripts)

- fill\_pole\_hole: fill observational hole at North pole (default: False)
- styleset: color style (e.g. "CMIP5")

Optional settings (variables)

• reference\_dataset: reference dataset

- 2. Script seaice\_trends.ncl
  - Required settings (scripts)
    - month: selected month (1, 2, ..., 12) or annual mean ("A")
    - region: region to be analyzed ( "Arctic" or "Antarctic")
  - Optional settings (scripts)
    - fill\_pole\_hole: fill observational hole at North pole, Default: False
  - Optional settings (variables)
    - ref\_model: array of references plotted as vertical lines
- 3. Script seaice\_tsline.ncl

Required settings (scripts)

• region: Arctic, Antarctic

• month: annual mean (A), or month number (3 = March, for Antarctic; 9 = September for Arctic)

Optional settings (scripts)

- styleset: for plot\_type cycle only (cmip5, cmip6, default)
- multi\_model\_mean: plot multi-model mean and standard deviation (default: False)
- EMs\_in\_lg: create a legend label for individual ensemble members (default: False)
- fill\_pole\_hole: fill polar hole (typically in satellite data) with sic = 1 (default: False)
- 4. Script seaice\_yod.ncl

Required settings (scripts)

- month: selected month (1, 2, ..., 12) or annual mean ("A")
- region: region to be analyzed ( "Arctic" or "Antarctic")

Optional settings (scripts)

- fill\_pole\_hole: fill observational hole at North pole, Default: False
- wgt\_file: netCDF containing pre-determined model weights

Optional settings (variables)

• ref\_model: array of references plotted as vertical lines

#### 21.9.4 Variables

- sic (ocean-ice, monthly mean, longitude latitude time)
- areacello (fx, longitude latitude)

#### 21.9.5 Observations and reformat scripts

Note: (1) obs4MIPs data can be used directly without any preprocessing; (2) use `esmvaltool data info DATASET` or see headers of cmorization scripts (in esmvaltool/cmorizers/data/formatters/datasets/) for non-obs4MIPs data for download instructions.

• HadISST (sic - esmvaltool/cmorizers/data/formatters/datasets/hadisst.ncl)

#### 21.9.6 References

- Massonnet, F. et al., The Cryosphere, 6, 1383-1394, doi: 10.5194/tc-6-1383-2012, 2012.
- Stroeve, J. et al., Geophys. Res. Lett., 34, L09501, doi:10.1029/2007GL029703, 2007.

#### 21.9.7 Example plots

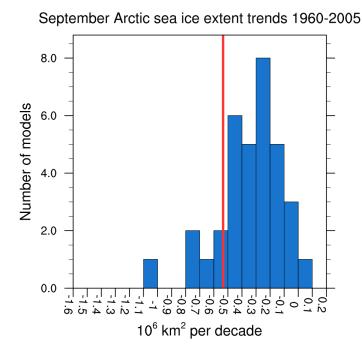


Fig. 5: Sea ice extent trend distribution for the Arctic in September (similar to IPCC AR5 Chapter 9, Fig. 9.24c). [seaice\_trends.ncl]

## 21.10 Seaice drift

#### 21.10.1 Overview

This recipe allows to quantify the relationships between Arctic sea-ice drift speed, concentration and thickness (Docquier et al., 2017). A decrease in concentration or thickness, as observed in recent decades in the Arctic Ocean (Kwok, 2018; Stroeve and Notz, 2018), leads to reduced sea-ice strength and internal stress, and thus larger sea-ice drift speed (Rampal et al., 2011). This in turn could provide higher export of sea ice out of the Arctic Basin, resulting in lower sea-ice concentration and further thinning. Olason and Notz (2014) investigate the relationships between Arctic sea-ice drift speed, concentration and thickness using satellite and buoy observations. They show that both seasonal and recent

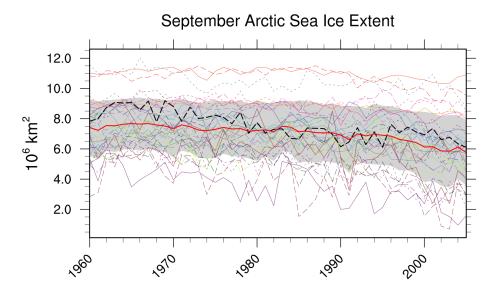


Fig. 6: Time series of total sea ice area and extent (accumulated) for the Arctic in September including multi-model mean and standard deviation (similar to IPCC AR5 Chapter 9, Fig. 9.24a). [seaice\_tsline.ncl]

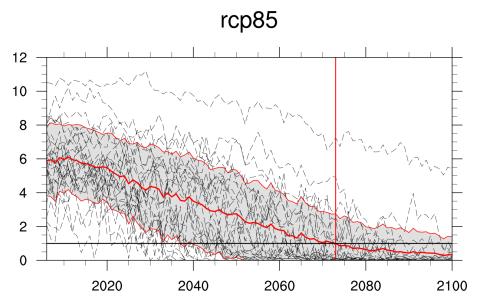


Fig. 7: Time series of September Arctic sea ice extent for individual CMIP5 models, multi-model mean and multi-model standard deviation, year of disappearance (similar to IPCC AR5 Chapter 12, Fig. 12.31e). [seaice\_yod.ncl]

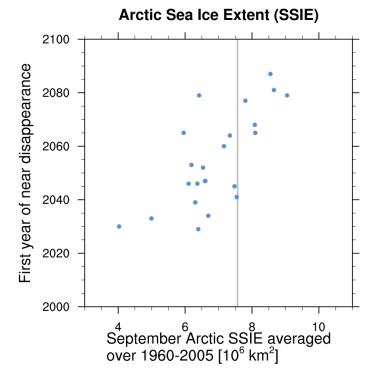


Fig. 8: Scatter plot of mean historical September Arctic sea ice extent vs 1st year of disappearance (RCP8.5) (similar to IPCC AR5 Chapter 12, Fig. 12.31a). [seaice\_ecs.ncl]

long-term changes in sea ice drift are primarily correlated to changes in sea ice concentration and thickness. This recipe allows to quantify these relationships in climate models.

In this recipe, four process-based metrics are computed based on the multi-year monthly mean sea-ice drift speed, concentration and thickness, averaged over the Central Arctic.

The first metric is the ratio between the modelled drift-concentration slope and the observed drift-concentration slope. The second metric is similar to the first one, except that sea-ice thickness is involved instead of sea-ice concentration. The third metric is the normalised distance between the model and observations in the drift-concentration space. The fourth metric is similar to the third one, except that sea-ice thickness is involved instead of sea-ice concentration.

#### 21.10.2 Available recipes and diagnostics

Recipes are stored in recipes/

• recipe\_seaice\_drift.yml

Diagnostics are stored in diag\_scripts/seaice\_drift/

• seaice\_drift.py: Compute metrics and plot results

#### 21.10.3 User settings in recipe

- 1. Script diag\_shapeselect.py
  - Required settings (scripts)

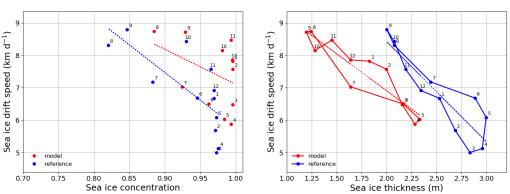
One of the following two combinations is required:

- 1. Latitude threshold:
  - latitude\_threshold: metric will be computed north of this latitude value
- 2. Polygon:
  - polygon: metric will be computed inside the give polygon. Polygon is defined as a list of (lon, lat) tuple
  - polygon\_name: name of the region defined by the polygon

#### 21.10.4 Variables

• sispeed, sithick, siconc (daily)

#### 21.10.5 Example plots



Seasonal cycle CMIP5\_GFDL-ESM2G\_historical\_r1i1p1\_1979\_2005

Scatter plots of modelled (red) and observed (blue) monthly mean sea-ice drift speed against sea-ice concentration (left panel) and sea-ice thickness (right panel) temporally averaged over the period 1979–2005 and spatially averaged over the SCICEX box.

## 21.11 Seaice feedback

#### 21.11.1 Overview

In this recipe, one process-based diagnostic named the Ice Formation Efficiency (IFE) is computed based on monthly mean sea-ice volume estimated north of 80°N. The choice of this domain is motivated by the desire to minimize the influence of dynamic processes but also by the availability of sea-ice thickness measurements. The diagnostic intends to evaluate the strength of the negative sea-ice thickness/growth feedback, which causes late-summer negative anomalies in sea-ice area and volume to be partially recovered during the next growing season. A chief cause behind the existence of this feedback is the non-linear inverse dependence between heat conduction fluxes and sea-ice thickness, which

implies that thin sea ice grows faster than thick sea ice. To estimate the strength of that feedback, anomalies of the annual minimum of sea-ice volume north of 80°N are first estimated. Then, the increase in sea-ice volume until the next annual maximum is computed for each year. The IFE is defined as the regression of this ice volume production onto the baseline summer volume anomaly.

#### 21.11.2 Available recipes and diagnostics

Recipes are stored in recipes/

• recipe\_seaice\_feedback.yml

Diagnostics are stored in diag\_scripts/seaice\_feedback/

• negative\_seaice\_feedback.py: scatterplot showing the feedback between seaice volume and seaice growth

#### 21.11.3 User settings

script negative\_seaice\_feedback.py

Optional settings for script

- plot: dictionary containing plot options:
  - point\_color: color of the plot points. (Default: black)
  - point\_size: size of the plot points. (Default: 10)
  - show\_values: show numerical values of feedback in plot. (Default: True)

#### 21.11.4 Variables

• sit (seaice, monthly mean, time latitude longitude)

#### 21.11.5 References

• Massonnet, F., Vancoppenolle, M., Goosse, H., Docquier, D., Fichefet, T. and Blanchard-Wrigglesworth, E., 2018. Arctic sea-ice change tied to its mean state through thermodynamic processes. Nature Climate Change, 8: 599-603.

#### 21.11.6 Example plots

#### 21.12 Shapeselect

#### 21.12.1 Overview

Impact modelers are often interested in data for irregular regions best defined by a shapefile. With the shapefile selector tool, the user can extract time series or CII data for a user defined region. The region is defined by a user provided shapefile that includes one or several polygons. For each polygon, a new timeseries, or CII, is produced with only one time series per polygon. The spatial information is reduced to a representative point for the polygon ('representative') or as an average of all grid points within the polygon boundaries ('mean\_inside'). If there are no grid points strictly inside the polygon, the 'mean\_inside' method defaults to 'representative' for that polygon. An option for displaying the grid points together with the shapefile polygon allows the user to assess which method is most optimal. In case

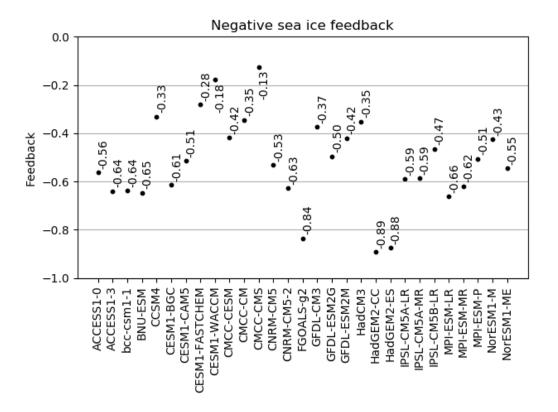


Fig. 9: Seaice negative feedback values (CMIP5 historical experiment 1979-2004).

interpolation to a high input grid is necessary, this can be provided in a pre-processing stage. Outputs are in the form of a NetCDF file, or as ascii code in csv format.

#### 21.12.2 Available recipes and diagnostics

Recipes are stored in recipes/

• recipe\_shapeselect.yml

Diagnostics are stored in diag\_scripts/shapeselect/

• diag\_shapeselect.py: calculate the average of grid points inside the user provided shapefile and returns the result as a NetCDF or Excel sheet.

#### 21.12.3 User settings in recipe

1. Script diag\_shapeselect.py

Required settings (scripts)

- shapefile: path to the user provided shapefile. A relative path is relative to the auxiliary\_data\_dir as configured in config-user.yml.
- weighting\_method: the preferred weighting method 'mean\_inside' mean of all grid points inside polygon; 'representative' one point inside or close to the polygon is used to represent the complete area.
- write\_xlsx: true or false to write output as Excel sheet or not.

• write\_netcdf: true or false to write output as NetCDF or not.

#### 21.12.4 Variables

• pr,tas (daily)

#### 21.12.5 Example plots

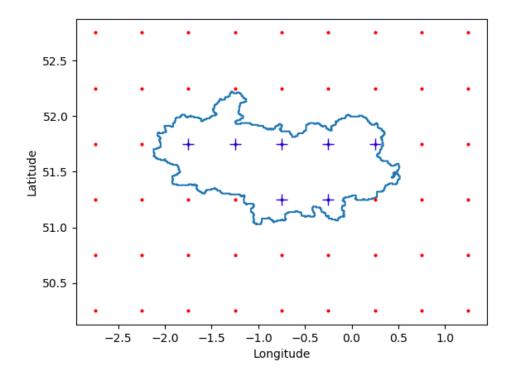


Fig. 10: Example of the selection of model grid points falling within (blue pluses) and without (red dots) a provided shapefile (blue contour).

# 21.13 Short test versions of scientific recipes to check for backward compatibility.

#### 21.13.1 Overview

These recipes are created to cover typical functionalities in the ESMValTool and allow to test them quickly. Each recipe should run less than 5 minutes to facilitate fast tests.

#### 21.13.2 Available recipes and diagnostics

Recipes are stored in recipes/testing/

• recipe\_deangelis15nat\_fig1\_fast.yml

Diagnostics are stored in diag\_scripts/

• deangelis15nat/deangelisf1b.py

Other recipes used for the continuous integration (CI) tests; these are run only by the automated tests:

• recipe\_python\_for\_CI.yml

This is identical to the example Python recipe, with the only difference being the location extraction preprocessor, which is replaced here with extract\_point. The reason for this is that this recipe is used solely for CI tests, and the geolocator/Nominatim engine for location extraction should not be used in CI runs as per their usage policy.

#### 21.13.3 User settings in recipes

The recipe recipe\_deangelis15nat\_fig1\_fast.yml calls the first diagnostic (deangelisf1b.py) from the original recipe recipe\_deangelis15nat.yml. It can be run with CMIP5 and CMIP6 models for any duration. Several flux variables (W m<sup>-2</sup>) and up to 6 different model experiments can be handled. Each variable needs to be given for each model experiment. The same experiments must be given for all models. For testing purpose it was reduce to two models, 3 experiments and one year. For a more detailed documentation see *Evaluate water vapor short wave radiance absorption schemes of ESMs with the observations*.

## 21.14 Toymodel

#### 21.14.1 Overview

The goal of this diagnostic is to simulate single-model ensembles from an observational dataset to investigate the effect of observational uncertainty. For further discussion of this synthetic value generator, its general application to forecasts and its limitations, see Weigel et al. (2008). The output is a netcdf file containing the synthetic observations. Due to the sampling of the perturbations from a Gaussian distribution, running the recipe multiple times, with the same observation dataset and input parameters, will result in different outputs.

#### 21.14.2 Available recipes and diagnostics

Recipes are stored in recipes/

• recipe\_toymodel.yml

Diagnostics are stored in diag\_scripts/magic\_bsc/

• toymodel.R: generates a single model ensemble of synthetic observations

#### 21.14.3 User settings

User setting files are stored in recipes/

1. recipe\_toymodel.yml

Required settings for preprocessor

extract\_region:

- start\_longitude: minimum longitude
- end\_longitude: maximum longitude
- start\_latitude: minimum longitude
- end\_latitude: maximum latitude

extract\_levels: (for 3D variables)

• levels: [50000] # e.g. for 500 hPa level

Required settings for script

- number\_of\_members: integer specifying the number of members to be generated
- beta: the user defined underdispersion (beta  $\geq 0$ )

#### 21.14.4 Variables

• any variable (atmos/ocean, daily-monthly, longitude, latitude, time)

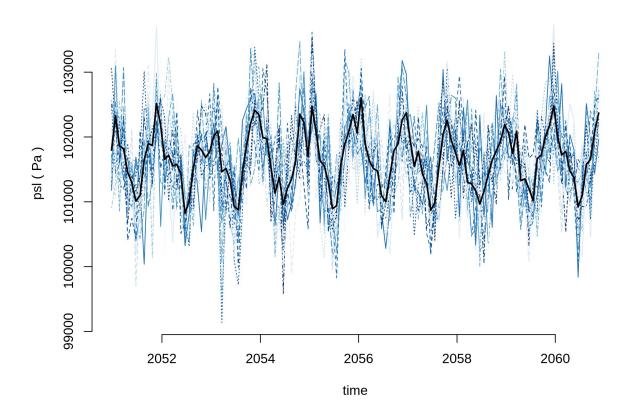
#### 21.14.5 Observations and reformat scripts

None

#### 21.14.6 References

- Bellprat, O., Massonnet, F., Siegert, S., Prodhomme, C., Macias-Gómez, D., Guemas, V., & Doblas-Reyes, F. (2017). Uncertainty propagation in observational references to climate model scales. Remote Sensing of Environment, 203, 101-108.
- Massonet, F., Bellprat, O. Guemas, V., & Doblas-Reyes, F. J. (2016). Using climate models to estimate the quality of global observational data sets. Science, aaf6369.
- Weigel, A. P., Liniger, M. A., & Appenzeller, C. (2008). Can multi-model combinations really enhance the prediction skill of probabilistic ensemble forecasts? Quarterly Journal of the Royal Meteorological Society, 134(630), 241-260.

#### 21.14.7 Example plots



20 synthetic members generated

Twenty synthetic single-model ensemble generated by the recipe\_toymodel.yml (see Section 3.7.2) for the 2051-2060 monthly data of r1i1p1 RCP 4.5 scenario of BCC\_CSM1-1 simulation.

## CHAPTER TWENTYTWO

## **BROKEN RECIPE LIST**

## 22.1 Broken recipe list

This table gives an overview of the recipes that are known to have issues. The table is always valid for the latest stable release of ESMValTool. More details can be found in the *broken recipe policy*.

Broken recipe	Affected diagnostics	Problem	GitHub issue	
recipe_check_obs.yml	ERA5_native6	Derivation of custom vari- ables <i>rlus</i> and <i>rsus</i>	#1388	
recipe_julia.yml	example	fill values are not inter- preted, resulting in an un- usable plot	#2595	
recipe_seaice_drift.yml	sea_ice_drift_SCICEX	shapely 2 issue	#3243	
recipe_pysplot.yml	plot_map	shapely 2 issue	#3483	

Table 1: Broken recip	es
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# Part VI

# **Obtaining input data**

ESMValTool supports input data from climate models participating in CMIP6, CMIP5, CMIP3, and CORDEX as well as observations, reanalysis, and any other data, provided that it adheres to the CF conventions and the data is described in a CMOR table as used in the various Climate Model Intercomparison Projects.

**Note:** CORDEX support is still work in progress. Contributions, in the form of *pull request reviews* or pull requests are most welcome. We are particularly interested in contributions from people with good understanding of the CORDEX project and its standards.

This section provides an introduction to getting (access to) climate data for use with ESMValTool.

Because the amount of data required by ESMValTool is typically large, it is recommended that you use the tool on a compute cluster where the data is already available, for example because it is connected to an ESGF node. Examples of such compute clusters are Levante and Jasmin, but many more exist around the world.

If you do not have access to such a facility through your institute or the project you are working on, you can request access by applying for the ENES Climate Analytics Service or, if you need longer term access or more computational resources, the IS-ENES3 Trans-national Access call.

If the options above are not available to you, ESMValTool also offers a feature to make it easy to download CMIP6, CMIP5, CMIP3, CORDEX, and obs4MIPs from ESGF. ESMValTool also provides support to download some observational dataset from source.

The chapter in the ESMValCore documentation on finding data explains how to configure ESMValTool so it can find locally available data and/or download it from ESGF if it isn't available locally yet.

## CHAPTER TWENTYTHREE

## MODELS

If you do not have access to a compute cluster with the data already mounted, ESMValTool can automatically download any required data that is available on ESGF. This is the recommended approach for first-time users to obtain some data for running ESMValTool. For example, run

esmvaltool run --search\_esgf=when\_missing examples/recipe\_python.yml

to run the default example recipe and automatically download the required data to the directory ~/climate\_data. The data only needs to be downloaded once, every following run will re-use previously downloaded data stored in this directory. See ESGF configuration for a more in depth explanation and the available configuration options.

Alternatively, you can use an external tool called Synda to maintain your own collection of ESGF data.

## CHAPTER TWENTYFOUR

## **OBSERVATIONS**

Observational and reanalysis products in the standard CF/CMOR format used in CMIP and required by ESMValTool are available via the obs4MIPs and ana4mips projects at the ESGF (e.g., https://esgf-data.dkrz.de/projects/esgf-dkrz/). Their use is strongly recommended, when possible.

Other datasets not available in these archives can be obtained by the user from the respective sources and reformatted to the CF/CMOR standard. ESMValTool currently supports two ways to perform this reformatting (aka 'CMORization'):

- 1. Using a CMORizer script: The first is to use a CMORizer script to generate a local pool of reformatted data that can readily be used by ESMValTool. This method is described in detail below.
- 2. Using fixes for on-the-fly CMORization: The second way is to implement specific 'fixes' for your dataset. In that case, the reformatting is performed 'on the fly' during the execution of an ESMValTool recipe (note that one of the first preprocessor tasks is 'CMOR checks and fixes'). Details on this second method are given at the *end of this chapter*.

A collection of readily CMORized OBS and OBS6 datasets can be accessed directly on CEDA/JASMIN and DKRZ. At CEDA/JASMIN OBS and OBS6 data is stored in the *esmeval* Group Workspace (GWS), and to be granted read (and execute) permissions to the GWS, one must apply at https://accounts.jasmin.ac.uk/services/group\_workspaces/ esmeval/; after permission has been granted, the user is encouraged to use the data locally, and not move it elsewhere, to minimize both data transfers and stale disk usage; to note that Tier 3 data is subject to data protection restrictions; for further inquiries, the GWS is administered by [Valeriu Predoi](mailto:valeriu.predoi@ncas.ac.uk).

## 24.1 Using a CMORizer script

ESMValTool comes with a set of CMORizers readily available. The CMORizers are dataset-specific scripts that can be run once to generate a local pool of CMOR-compliant data. The necessary information to download and process the data is provided in the header of each CMORizing script. These scripts also serve as template to create new CMORizers for datasets not yet included. Note that datasets CMORized for ESMValTool v1 may not be working with v2, due to the much stronger constraints on metadata set by the iris library.

ESMValTool provides the esmvaltool data command line tool, which can be used to download and format datasets.

To list the available commands, run

esmvaltool data --help

It is also possible to get help on specific commands, e.g.

esmvaltool data download --help

The list of datasets supported by ESMValTool through a CMORizer script can be obtained with:

esmvaltool data list

Datasets for which auto-download is supported can be downloaded with:

esmvaltool data download --config\_file [CONFIG\_FILE] [DATASET\_LIST]

Note that all Tier3 and some Tier2 datasets for which auto-download is supported will require an authentication. In such cases enter your credentials in your ~/.netrc file as explained here.

An entry to the ~/.netrc should look like:

machine [server\_name] login [user\_name] password [password]

Make sure that the permissions of the ~/.netrc file are set so only you and administrators can read it, i.e.

```
chmod 600 ~/.netrc
ls -l ~/.netrc
```

The latter command should show -rw-----.

For other datasets, downloading instructions can be obtained with:

```
esmvaltool data info [DATASET]
```

To CMORize one or more datasets, run:

```
esmvaltool data format --config_file [CONFIG_FILE] [DATASET_LIST]
```

The path to the raw data to be CMORized must be specified in the *user configuration file* as RAWOBS. Within this path, the data are expected to be organized in subdirectories corresponding to the data tier: Tier2 for freely-available datasets (other than obs4MIPs and ana4mips) and Tier3 for restricted datasets (i.e., dataset which requires a registration to be retrieved or provided upon request to the respective contact or PI). The CMORization follows the CMIP5 CMOR tables or CMIP6 CMOR tables for the OBS and OBS6 projects respectively. The resulting output is saved in the output\_dir, again following the Tier structure. The output file names follow the definition given in config-developer file for the OBS project:

[project]\_[dataset]\_[type]\_[version]\_[mip]\_[short\_name]\_YYYYMM\_YYYYMM.nc

where project may be OBS (CMIP5 format) or OBS6 (CMIP6 format), type may be sat (satellite data), reanaly (reanalysis data), ground (ground observations), clim (derived climatologies), campaign (aircraft campaign).

At the moment, esmvaltool data format supports Python and NCL scripts.

### 24.2 Supported datasets for which a CMORizer script is available

A list of the datasets for which a CMORizers is available is provided in the following table.

Dataset	Variables (MIP)	Tier	Script language
AGCD	pr (Amon)	2	Python
APHRO-MA	pr, tas (day), pr, tas (Amon)	3	Python
AURA-TES	tro3 (Amon)	3	NCL
BerkelyEarth	tas, tasa (Amon), sftlf (fx)	2	Python

continues on next page

Dataset	Variables (MIP)	Tier	Script language
CALIPSO-GOCCP	clcalipso (cfMon)	2	NCL
CALIPSO-	cli (AMon)	3	NCL
ICECLOUD			
CDS-SATELLITE-	bdalb (Lmon), bhalb (Lmon)	3	Python
ALBEDO			
CDS-SATELLITE-	fapar (Lmon), lai (Lmon)	3	Python
LAI-FAPAR	(1)	2	NOI
CDS-SATELLITE-	sm (day), sm (Lmon)	3	NCL
SOIL-MOISTURE	am (Eéhr)	2	Druthan
CDS-UERRA CDS-XCH4	sm (E6hr) xch4 (Amon)	3 3	Python NCL
CDS-XCO2	xco2 (Amon)	3	NCL
CERES-EBAF	rlut, rlutcs, rsut, rsutcs (Amon)	2	Python
CERES-SYN1deg	rlds, rldscs, rlus, rluscs, rlut, rlutcs, rsds, rs-	3	NCL
CLICLS STITLING	dscs, rsus, rsuscs, rsut, rsutcs (3hr) rlds, rld-	5	NeL
	scs, rlus, rlut, rlutcs, rsds, rsdt, rsus, rsut,		
	rsutes (Amon)		
CLARA-AVHRR	clt, clivi, clwvi, lwp (Amon)	3	NCL
CLOUDSAT-L2	clw, clivi, clwvi, lwp (Amon)	3	NCL
CowtanWay	tasa (Amon)	2	Python
CRU	tas, pr (Amon)	2	Python
CT2019	co2s (Amon)	2	Python
Duveiller2018	albDiffiTr13	2	Python
E-OBS	tas, tasmin, tasmax, pr, psl (day, Amon)	2	Python
Eppley-VGPM- MODIS	intpp (Omon)	2	Python
ERA5 <sup>1</sup>	cl, clt, evspsbl, evspsblpot, mrro, pr, prsn, ps, psl, ptype, rls, rlds, rlns, rlus <sup>2</sup> , rsds, rsns, rsus <sup>Page 497, 2</sup> , rsdt, rss, uas, vas, tas, tasmax, tasmin, tdps, ts, tsn (E1hr/Amon), orog (fx)	3	n/a
ERA5-Land <sup>Page 497, 1</sup>	pr	3	n/a
ERA-Interim	cl, cli, clivi, clt, clw, clwvi, evspsbl, hfds,	3	Python
	hur, hus, lwp, orog, pr, prsn, prw, ps, psl, rlds, rlut, rlutcs, rsds, rsdt, rss, rsut, rsutcs, sftlf, ta, tas, tasmax, tasmin, tauu, tauv, tdps, tos, ts, tsn, ua, uas, va, vas, wap, zg		
ERA-Interim-Land	sm (Lmon)	3	Python
ESACCI-AEROSOL	abs550aer, od550aer, od550aerStderr, od550lt1aer, od870aer, od870aerStderr (aero)	2	NCL
ESACCI-CLOUD	clivi, clt, cltStderr, clwvi, lwp, rlut, rlutcs, rsut, rsutcs, rsdt, rlus, rsus, rsuscs (Amon)	2	NCL
ESACCI-FIRE	burntArea (Lmon)	2	NCL
ESACCI-	baresoilFrac, cropFrac, grassFrac,	2	NCL
LANDCOVER	shrubFrac, treeFrac (Lmon)		
ESACCI-LST	ts (Amon)	2	Python
ESACCI-OC	chl (Omon)	2	Python
ESACCI-OZONE	toz, tozStderr, tro3prof, tro3profStderr (Amon)	2	NCL

Table 1 – continued from previous pag	е
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Dataset	Variables (MIP)	Tier	Script language
ESACCI-SEA- SURFACE- SALINITY	sos (Omon)	2	Python
ESACCI- SOILMOISTURE	dos, dosStderr, sm, smStderr (Lmon)	2	NCL
ESACCI-SST	ts, tsStderr (Amon)	2	NCL
ESACCI- WATERVAPOUR	prw (Amon)	3	Python
ESDC	tas, tasmax, tasmin (Amon)	2	Python
ESRL	co2s (Amon)	2	NCL
FLUXCOM	gpp (Lmon)	3	Python
GCP2018	fgco2 (Omon <sup>3</sup> ), nbp (Lmon <sup>Page 497, 3</sup> )	2	Python
GCP2020	fgco2 (Omon <sup>Page 497, 3</sup> ), nbp (Lmon <sup>Page 497, 3</sup> )	2	Python
GHCN	pr (Amon)	2	NCL
GHCN-CAMS	tas (Amon)	2	Python
GISTEMP	tasa (Amon)	2	Python
GLODAP	dissic, ph, talk (Oyr)	2	Python
GPCC	pr (Amon)	2	Python
GPCP-SG	pr (Amon)	2	Python
GRACE	lweGrace (Lmon)	3	Python
HadCRUT3	tas, tasa (Amon)	2	NCL
HadCRUT4	tas, tasa (Amon), tasConf5, tasConf95	2	NCL
HadCRUT5	tas, tasa (Amon)	2	Python
HadISST	sic (OImon), tos (Omon), ts (Amon)	2	NCL
HALOE	tro3, hus (Amon)	2	NCL
HWSD	cSoil (Lmon), areacella (fx), sftlf (fx)	3	Python
ISCCP-FH	alb, prw, ps, rlds, rlus, rlut, rlutcs, rsds, rsdt, rsus, rsut, rsutcs, tas, ts (Amon)	2	NCL
JMA-TRANSCOM	nbp (Lmon), fgco2 (Omon)	3	Python
JRA-25	clt, hus, prw, rlut, rlutcs, rsut, rsutcs (Amon)	2	Python
Kadow2020	tasa (Amon)	2	Python
LAI3g	lai (Lmon)	3	Python
LandFlux-EVAL	et, etStderr (Lmon)	3	Python
Landschuetzer2016	dpco2, fgco2, spco2 (Omon)	2	Python
Landschuetzer2020	spco2 (Omon)	2	Python
MAC-LWP	lwp, lwpStderr (Amon)	3	NCL
MERRA	cli, clivi, clt, clw, clwvi, hur, hus, lwp, pr, prw, ps, psl, rlut, rlutcs, rsdt, rsut, rsutcs, ta, tas, ts, ua, va, wap, zg (Amon)	3	NCL
MERRA2	sm (Lmon) clt, pr, evspsbl, hfss, hfls, huss, prc, prsn, prw, ps, psl, rlds, rldscs, rlus, rlut, rlutcs, rsds, rsdscs, rsdt, tas, tasmin, tas- max, tauu, tauv, ts, uas, vas, rsus, rsuscs, rsut, rsutcs, ta, ua, va, tro3, zg, hus, wap, hur, cl, clw, cli, clwvi, clivi (Amon)	3	Python
MLS-AURA	hur, hurStderr (day)	3	Python
MOBO-DIC_MPIM	dissic (Omon)	2	Python

Table	1 - continued	from previous page
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Dataset	Variables (MIP)	Tier	Script language
MOBO-DIC2004- 2019	dissic (Omon)	2	Python
MODIS	cliwi, clt, clwvi, iwpStderr, lwpStderr (Amon), od550aer (aero)	3	NCL
MSWEP <sup>Page 497, 1</sup>	pr	3	n/a
MTE	gpp, gppStderr (Lmon)	3	Python
NCEP-NCAR-R1	clt, hur, hurs, hus, pr, prw, psl, rlut, rlutcs, rsut, rsutcs, sfcWind, ta, tas, tasmax, tas- min, ts, ua, va, wap, zg (Amon) pr, rlut, ua, va (day)	2	Python
NCEP-DOE-R2	clt, hur, prw, ta, wap (Amon)	2	Python
NDP	cVeg (Lmon)	3	Python
NIWA-BS	toz, tozStderr (Amon)	3	NCL
NOAA-CIRES- 20CR-V2	clt, clwvi, hus, prw, rlut, rsut (Amon)	2	Python
NOAA-CIRES- 20CR-V3	clt, clwvi, hus, prw, rlut, rlutcs, rsut, rsutcs (Amon)	2	Python
NOAA-ERSSTv3b	tos (Omon)	2	Python
NOAA-ERSSTv5	tos (Omon)	2	Python
NOAA-MBL-CH4	ch4s (Amon)	2	Python
NOAAGlobalTemp	tasa (Amon)	2	Python
NSIDC-0116- $[nh sh]^4$	usi, vsi (day)	3	Python
NSIDC-g02202-[sh]	siconc (SImon)	3	Python
OceanSODA-ETHZ	areacello (Ofx), co3os, dissicos, fgco2, phos, spco2, talkos (Omon)	2	Python
OSI-450-[nh sh]	sic (OImon), sic (day)	2	Python
PATMOS-x	clt (Amon)	2	NCL
PERSIANN-CDR	pr (Amon), pr (day)	2	Python
PHC	thetao, so (Omon <sup>3</sup> )	2	Python
PIOMAS	sit (day)	2	Python
REGEN	pr (day, Amon)	2	Python
Scripps-CO2-KUM	co2s (Amon)	2	Python
TCOM-CH4	ch4 (Amon <sup>3</sup> )	2	Python
TCOM-N2O	n2o (Amon <sup>3</sup> )	2	Python
UWisc	clwvi, lwpStderr (Amon)	3	NCL
WFDE5	tas, pr (Amon, day)	2	Python
WOA	thetao, so, tos, sos (Omon) no3, o2, po4, si (Oyr)	2	Python

Table 1 – continued from previous page

<sup>&</sup>lt;sup>1</sup> CMORization is built into ESMValTool through the native6 project, so there is no separate CMORizer script.

<sup>&</sup>lt;sup>2</sup> Derived on the fly from down & net radiation.

<sup>&</sup>lt;sup>3</sup> The frequency of this variable differs from the one specified in the table. The correct entry that needs to be used in the recipe can be found in the corresponding section of recipe\_check\_obs.yml.

<sup>&</sup>lt;sup>4</sup> The cmoriser requires PROJ>=9.3. Previous version of PROJ will return an error: Internal Proj Error: proj\_create: unhandled axis direction: UNKNOWN) You can check the version of PROJ in your conda environment by running: conda list PROJ.

CHAPTER TWENTYFIVE

# DATASETS IN NATIVE FORMAT

ESMValCore also provides support for some datasets in their native format. In this case, the steps needed to reformat the data are executed as dataset fixes during the execution of an ESMValTool recipe, as one of the first preprocessor steps, see fixing data. Compared to the workflow described above, this has the advantage that the user does not need to store a duplicate (CMORized) copy of the data. Instead, the CMORization is performed 'on the fly' when running a recipe. Native datasets can be hosted either under a dedicated project (usually done for native model output) or under project native6 (usually done for native reanalysis/observational products). These projects are configured in the config-developer file.

A list of all currently supported native datasets is provided here. A detailed description of how to include new native datasets is given here.

To use this functionality, users need to provide a path in the User configuration file for the native6 project data and/or the dedicated project used for the native dataset, e.g., ICON. Then, in the recipe, they can refer to those projects. For example:

```
datasets:
- {project: native6, dataset: ERA5, type: reanaly, version: v1, tier: 3, start_year:_
- 1990, end_year: 1990}
- {project: ICON, dataset: ICON, exp: icon-2.6.1_atm_amip_R2B5_r1i1p1f1, mip: Amon,_
- short_name: tas, start_year: 2000, end_year: 2014}
```

For project native6, more examples can be found in the diagnostics ERA5\_native6 in the recipe examples/recipe\_check\_obs.yml.

# Part VII

# Making a recipe or diagnostic

# CHAPTER TWENTYSIX

# INTRODUCTION

This chapter contains instructions for developing your own recipes and/or diagnostics. It also contains a section describing how to use additional datasets with ESMValTool. While it is possible to use just the ESMValCore package and run any recipes/diagnostics you develop with just this package, it is highly recommended that you consider contributing the work you do back to the ESMValTool community. Among the advantages of contributing to the community are improved visibility of your work and support by the community with making and maintaining your diagnostic. See the *Community* chapter for a guide on how to contribute to the community.

# CHAPTER TWENTYSEVEN

# RECIPE

# 27.1 Writing a basic recipe

The user will need to write a basic recipe to be able to run their own personal diagnostic. An example of such a recipe is found in *esmvaltool/recipes/recipe\_my\_personal\_diagnostic.yml*. For general guidelines with regards to ESMValTool recipes please consult the User Guide; the specific parameters needed by a recipe that runs a personal diagnostic are:

```
scripts:
    my_diagnostic:
    script: /path/to/your/my_little_diagnostic.py
```

i.e. the full path to the personal diagnostic that the user needs to run.

There is also a lesson available in the ESMValTool tutorial that describes in a step-by-step procedure how to write your own recipe. It can be found here.

# CHAPTER TWENTYEIGHT

# DIAGNOSTIC

# 28.1 Instructions for personal diagnostic

Anyone can run a personal diagnostic, no matter where the location of it; there is no need to install esmvaltool in developer mode nor is it to git push or for that matter, do any git operations; the example recipe

esmvaltool/recipes/recipe\_my\_personal\_diagnostic.yml

shows the use of running a personal diagnostic; the example

esmvaltool/diag\_scripts/examples/my\_little\_diagnostic.py

and any of its alterations may be used as training wheels for the future ESMValTool diagnostic developer. The purpose of this example is to familiarize the user with the framework of ESMValTool without the constraints of installing and running the tool as developer.

# 28.2 Functionality

*my\_little\_diagnostic* (or whatever the user will call their diagnostic) makes full use of ESMValTool's preprocessor output (both phyisical files and run variables); this output comes in form of a nested dictionary, or config dictionary, see an example below; it also makes full use of the ability to call any of the preprocessor's functions, note that relative imports of modules from the esmvaltool package are allowed and work without altering the \$PYTHONPATH.

The user may parse this dictionary so that they execute a number of operations on the preprocessed data; for example the *my\_little\_diagnostic.plot\_time\_series* grabs the preprocessed data output, computes global area averages for each model, then plots a time-series for each model. Different manipulation functionalities for grouping, sorting etc of the data in the config dictionary are available, please consult ESMValTool User Manual.

# 28.3 Example of config dictionary

To be added (use python-style code-block).

CHAPTER

## TWENTYNINE

# WRITING A CMORIZER SCRIPT FOR AN ADDITIONAL DATASET

ESMValTool is designed to work with CF compliant data and follows the CMOR tables from the CMIP data request, therefore the observational datasets need to be CMORized for usage in ESMValTool. The following steps are necessary to prepare an observational data set for the use in ESMValTool.

- 1. Check if your variable is CMOR standard
- 2. Edit your configuration file
- 3. Store your dataset in the right place
- 3.1 Downloader script (optional)
- *4. Create a cmorizer for the dataset*
- 4.1 Cmorizer script written in python
- 4.2 Cmorizer script written in NCL
- 5. Run the cmorizing script
- 6. Naming convention of the observational data files
- 7. Test the cmorized dataset

**Note:** CMORization as a fix. As of early 2020, we've started implementing cmorization as *fixes*. As compared to the workflow described below, this has the advantage that the user does not need to store a duplicate (CMORized) copy of the data. Instead, the CMORization is performed 'on the fly' when running a recipe. **ERA5** is the first dataset for which this 'CMORization on the fly' is supported. For more information, see *Datasets in native format*.

# 29.1 1. Check if your variable is CMOR standard

Most variables are defined in the CMIP data request and can be found in the CMOR tables in the folder /esmvalcore/cmor/tables/cmip6/Tables/, differentiated according to the MIP they belong to. The tables are a copy of the PCMDI guidelines. If you find the variable in one of these tables, you can proceed to the next section.

If your variable is not available in the standard CMOR tables, you need to write a custom CMOR table entry for the variable as outlined below and add it to /esmvalcore/cmor/tables/custom/.

To create a new custom CMOR table you need to follow these guidelines:

- Provide the variable\_entry;
- Provide the modeling\_realm;

- Provide the variable attributes, but leave standard\_name blank. Necessary variable attributes are: units, cell\_methods, cell\_measures, long\_name, comment.
- Provide some additional variable attributes. Necessary additional variable attributes are: dimensions, out\_name, type. There are also additional variable attributes that can be defined here (see the already available cmorizers).

It is recommended to use an existing custom table as a template, to edit the content and save it as CMOR\_<short\_name>. dat.

# 29.2 2. Edit your configuration file

Make sure that beside the paths to the model simulations and observations, also the path to raw observational data to be cmorized (RAWOBS) is present in your configuration file.

# 29.3 3. Store your dataset in the right place

The folder RAWOBS needs the subdirectories Tier1, Tier2 and Tier3. The different tiers describe the different levels of restrictions for downloading (e.g. providing contact information, licence agreements) and using the observations. The unformatted (raw) observations should then be stored in the appropriate of these three folders.

For each additional dataset, an entry needs to be made to the file datasets.yml. The dataset entry should contain:

- the correct tier information;
- the source of the raw data;
- the last\_access date;
- the info that explain how to download the data.

Note that these fields should be identical to the content of the header of the cmorizing script (see Section 4. *Create a cmorizer for the dataset*).

## 29.3.1 3.1 Downloader script (optional)

A Python script can be written to download raw observations from source and store the data in the appropriate tier subdirectory of the folder RAWOBS automatically. There are many downloading scripts available in /esmval-tool/cmorizers/data/downloaders/datasets/ where several data download mechanisms are provided:

- A wget get based downloader for http(s) downloads, with a specific derivation for NASA datasets.
- A *ftp* downloader with a specific derivation for ESACCI datasets available from CEDA.
- A Climate Data Store downloader based on *cdsapi*.

Note that the name of this downloading script has to be identical to the name of the dataset.

Depending on the source server, the downloading script needs to contain paths to raw observations, filename patterns and various necessary fields to retrieve the data. Default start\_date and end\_date can be provided in cases where raw data are stored in daily, monthly, and yearly files.

The downloading script for the given dataset can be run with:

```
esmvaltool data download --config_file <config-user.yml> <dataset-name>
```

The options --start and --end can be added to the command above to restrict the download of raw data to a time range. They will be ignored if a specific dataset does not support it (i.e. because it is provided as a single file). Valid formats are YYYY, YYYYMM and YYYYMMDD. By default, already downloaded data are not overwritten unless the option --overwrite=True is used.

# 29.4 4. Create a cmorizer for the dataset

There are many cmorizing scripts available in /esmvaltool/cmorizers/data/formatters/datasets/ where solutions to many kinds of format issues with observational data are addressed. These scripts are either written in Python or in NCL.

Note: NCL support will terminate soon, so new cmorizer scripts should preferably be written in Python.

How much emorizing an observational data set needs is strongly dependent on the original NetCDF file and how close the original formatting already is to the strict CMOR standard.

In the following two subsections two emorizing scripts, one written in Python and one written in NCL, are explained in more detail.

### 29.4.1 4.1 Cmorizer script written in python

Find here an example of a cmorizing script, written for the MTE dataset that is available at the MPI for Biogeochemistry in Jena: mte.py.

All the necessary information about the dataset to write the filename correctly, and which variable is of interest, is stored in a separate configuration file: MTE.yml in the directory ESMValTool/esmvaltool/cmorizers/data/ cmor\_config/. Note that both the name of this configuration file and the cmorizing script have to be identical to the name of your dataset. It is recommended that you set project to OBS6 in the configuration file. That way, the variables defined in the CMIP6 CMOR table, augmented with the custom variables described above, are available to your script.

The first part of this configuration file defines the filename of the raw observations file. The second part defines the common global attributes for the cmorizer output, e.g. information that is needed to piece together the final observations file name in the correct structure (see Section 6. Naming convention of the observational data files). Another global attribute is reference which includes a doi related to the dataset. Please see the section adding references on how to add reference tags to the reference section in the configuration file. If a single dataset has more than one reference, it is possible to add tags as a list e.g. reference: ['tag1', 'tag2']. The third part in the configuration file defines the variables that are supposed to be emorized.

The actual cmorizing script mte.py consists of a header with information on where and how to download the data, and noting the last access of the data webpage.

The main body of the CMORizer script must contain a function called

def cmorization(in\_dir, out\_dir, cfg, cfg\_user, start\_date, end\_date):

with this exact call signature. Here, in\_dir corresponds to the input directory of the raw files, out\_dir to the output directory of final reformatted data set, cfg to the dataset-specific configuration file, cfg\_user to the user configuration file, start\_date to the start of the period to format, and end\_date to the end of the period to format. If not needed, the last three arguments can be ignored using underscores. The return value of this function is ignored. All the work, i.e. loading of the raw files, processing them and saving the final output, has to be performed inside its body. To simplify this process, ESMValTool provides a set of predefined utilities.py, which can be imported into your CMORizer by

#### from esmvaltool.cmorizers.data import utilities as utils

Apart from a function to easily save data, this module contains different kinds of small fixes to the data attributes, coordinates, and metadata which are necessary for the data field to be CMOR-compliant.

Note that this specific CMORizer script contains several subroutines in order to make the code clearer and more readable (we strongly recommend to follow that code style). For example, the function \_get\_filepath converts the raw filepath to the correct one and the function \_extract\_variable extracts and saves a single variable from the raw data.

#### 29.4.2 4.2 Cmorizer script written in NCL

Find here an example of a cmorizing script, written for the ESACCI XCH4 dataset that is available on the Copernicus Climate Data Store: cds\_xch4.ncl.

The first part of the script collects all the information about the dataset that are necessary to write the filename correctly and to understand which variable is of interest here. Please make sure to provide the correct information for following key words: DIAG\_SCRIPT, VAR, NAME, MIP, FREQ, CMOR\_TABLE.

- Note: the fields VAR, NAME, MIP and FREQ all ask for one or more entries. If more than one entry is provided, make sure that the order of the entries is the same for all four fields! (for example, that the first entry in all four fields describe the variable xch4 that you would like to extract);
- Note: some functions in the script are NCL-specific and are available through the loading of the script interface.ncl. There are similar functions available for python scripts.

In the second part of the script each variable defined in VAR is separately extracted from the original data file and processed. Most parts of the code are commented, and therefore it should be easy to follow. ESMValTool provides a set of predefined utilities.ncl, which are imported by default into your CMORizer. This module contains different kinds of small fixes to the data attributes, coordinates, and metadata which are necessary for the data field to be CMOR-compliant.

## 29.5 5. Run the cmorizing script

The cmorizing script for the given dataset can be run with:

esmvaltool data format --config\_file <config-user.yml> <dataset-name>

The options --start and --end can be added to the command above to restrict the formatting of raw data to a time range. They will be ignored if a specific dataset does not support it (i.e. because it is provided as a single file). Valid formats are YYYY, YYYYMM and YYYYMDD.

**Note:** The output path given in the configuration file is the path where your cmorized dataset will be stored. The ESMValTool will create a folder with the correct tier information (see Section 2. *Edit your configuration file*) if that tier folder is not already available, and then a folder named after the dataset. In this folder the cmorized data set will be stored as a NetCDF file. The cmorized dataset will be automatically moved to the correct tier subfolder of your OBS6 directory if the option --install=True is used in the command above and no such directory was already created.

If your run was successful, one or more NetCDF files are produced in your output directory.

If a downloading script is available for the dataset, the downloading and the cmorizing scripts can be run in a single command with:

esmvaltool data prepare --config\_file <config-user.yml> <dataset-name>

Note that options from the `esmvaltool data download and esmvaltool data format commands can be passed to the above command.

## 29.6 6. Naming convention of the observational data files

For the ESMValTool to be able to read the observations from the NetCDF file, the file name needs a very specific structure and order of information parts (very similar to the naming convention for observations in ESMValTool v1.0). The file name will be automatically correctly created if a cmorizing script has been used to create the netCDF file.

The correct structure of an observational data set is defined in config-developer.yml, and looks like the following:

OBS\_[dataset]\_[type]\_[version]\_[mip]\_[short\_name]\_YYYYMM-YYYYMM.nc

For the example of the CDS-XCH4 data set, the correct structure of the file name looks then like this:

OBS\_CDS-XCH4\_sat\_L3\_Amon\_xch4\_200301-201612.nc

The different parts of the name are explained in more detail here:

- OBS: describes what kind of data can be expected in the file, in this case observations;
- CDS-XCH4: that is the name of the dataset. It has been named this way for illustration purposes (so that everybody understands it is the xch4 dataset downloaded from the CDS), but a better name would indeed be ESACCI-XCH4 since it is a ESA-CCI dataset;
- sat: describes the source of the data, here we are looking at satellite data (therefore sat), could also be reanaly for reanalyses;
- L3: describes the version of the dataset:
- Amon: is the information in which mip the variable is to be expected, and what kind of temporal resolution it has; here we expect xch4 to be part of the atmosphere (A) and we have the dataset in a monthly resolution (mon);
- xch4: Is the name of the variable. Each observational data file is supposed to only include one variable per file;
- 200301-201812: Is the period the dataset spans with 200301 being the start year and month, and 201812 being the end year and month;

**Note:** There is a different naming convention for obs4MIPs data (see the exact specifications for the obs4MIPs data file naming convention in the config-developer.yml file).

## 29.7 7. Test the cmorized dataset

To verify that the cmorized data file is indeed correctly formatted, you can run a dedicated test recipe, that does not include any diagnostic, but only reads in the data file and has it processed in the preprocessor. Such a recipe is called recipes/examples/recipe\_check\_obs.yml. You just need to add a diagnostic for your dataset following the existing entries. Only the diagnostic of interest needs to be run, the others should be commented out for testing.

# Part VIII

# **Contributing to the community**

#### Contributions are very welcome!

This chapter explains how to contribute to ESMValTool. We greatly value contributions of any kind. Contributions could include, but are not limited to documentation improvements, bug reports, new or improved diagnostic code, scientific and technical code reviews, infrastructure improvements, maintenance of recipes, mailing list and chat participation, community help/building, education and outreach.

If you have a bug or other issue to report, please open an issue on the issues tab on the ESMValTool github repository.

In case anything is unclear feel free to contact us for more information and help, e.g. on our GitHub Discussions page.

CHAPTER

THIRTY

# **CONTRIBUTING CODE AND DOCUMENTATION**

If you would like to contribute a new diagnostic and recipe or a new feature, please discuss your idea with the development team before getting started, to avoid double work and/or disappointment later. A good way to do this is to open an issue on GitHub. This is also a good way to get help with the implementation.

We value the time you invest in contributing and strive to make the process as easy as possible. If you have suggestions for improving the process of contributing, please do not hesitate to propose them, for example by starting a discussion on our discussions page.

## 30.1 Getting started

See Install from source for instructions on how to set up a development installation.

New development should preferably be done in the ESMValTool GitHub repository. However, for scientists requiring confidentiality, private repositories are available, see *Moving work from the private to the public repository* for more information. The default git branch is main. Use this branch to create a new feature branch from and make a pull request against. This page offers a good introduction to git branches, but it was written for BitBucket while we use GitHub, so replace the word BitBucket by GitHub whenever you read it.

It is recommended that you open a draft pull request early, as this will cause *CircleCI to run the unit tests*, *Codacy to analyse your code*, and *readthedocs to build the documentation*. It's also easier to get help from other developers if your code is visible in a pull request.

Please review the results of the automatic checks below your pull request. If one of the tests shows a red cross instead of a green checkmark, please click the Details link behind the failing check and try to solve the issue. Ask @ESMValGroup/tech-reviewers for help if you do not know how to fix the failing check. Note that this kind of automated checks make it easier to *review code*, but they are not flawless. Preferably Codacy code quality checks pass, however a few remaining hard to solve Codacy issues are still acceptable. If you suspect Codacy may be wrong, please ask by commenting on your pull request.

## 30.2 Checklist for pull requests

To clearly communicate up front what is expected from a pull request, we have the following checklist. Please try to do everything on the list before requesting a review. If you are unsure about something on the list, please ask the @ESMValGroup/tech-reviewers or @ESMValGroup/science-reviewers for help by commenting on your (draft) pull request or by starting a new discussion.

In the ESMValTool community we use *pull request reviews* to ensure all code and documentation contributions are of good quality. The icons indicate whether the item will be checked during the *Technical review* or *Scientific review*.

### 30.2.1 All pull requests

- The pull request has a descriptive title
- Code is written according to the code quality guidelines
- Documentation is available
- Tests run successfully
- The *list of authors* is up to date
- Changed dependencies are added or removed correctly
- The checks shown below the pull request are successful

If a pull request introduces a change that causes a recipe to no longer run successfully (*breaking change*), or which results in scientifically significant changes in results (*science change*), additional requirements defined in the *backward compatibility policy* apply. These include in particular:

- Instructions for the release notes to assist *recipe developers* to adapt their recipe in light of the *backward-incompatible change* available.
- If applicable, instructions for *recipe developers* working on *user recipes* to enable them to adapt their code related to *backward-incompatible changes* available (see ESMValTool\_Tutorial: issue #263) available.
- Core development team tagged to notify them of the *backward-incompatible change*, and give at least 2 weeks for objections to be raised before merging to the main branch. If a strong objection is raised the backward-incompatible change should not be merged until the objection is resolved.
- Information required for the "*backward-incompatible changes*" section in the PR that introduces the *backward-incompatible change* available.

## 30.2.2 New or updated recipe and/or diagnostic

See Making a new diagnostic or recipe for detailed instructions.

- Recipe runs successfully
- *Recipe and diagnostic documentation* is available
- *Figure(s) and data* look as expected from literature
- Provenance information has been added

## 30.2.3 New or updated data reformatting script

See *new dataset* for detailed instructions.

- *Dataset documentation* is available
- The dataset has been *added to the CMOR check recipe*
- Numbers and units of the data look physically meaningful

## 30.3 Pull request title

The title of a pull request should clearly describe what the pull request changes. If you need more text to describe what the pull request does, please add it in the description. The titles of pull requests are used to compile the *Changelog*, therefore it is important that they are easy to understand for people who are not familiar with the code or people in the project. Descriptive pull request titles also makes it easier to find back what was changed when, which is useful in case a bug was introduced.

# 30.4 Code quality

To increase the readability and maintainability or the ESMValTool source code, we aim to adhere to best practices and coding standards. For code in all languages, it is highly recommended that you split your code up in functions that are short enough to view without scrolling, e.g. no more than 50 lines long.

We include checks for Python, R, NCL, and yaml files, most of which are described in more detail in the sections below. This includes checks for invalid syntax and formatting errors. *Pre-commit* is a handy tool that can run all of these checks automatically just before you commit your code. It knows knows which tool to run for each filetype, and therefore provides a convenient way to check your code.

## 30.4.1 Python

The standard document on best practices for Python code is PEP8 and there is PEP257 for code documentation. We make use of numpy style docstrings to document Python functions that are visible on readthedocs.

To check if your code adheres to the standard, go to the directory where the repository is cloned, e.g. cd ESMValTool, and run prospector

prospector esmvaltool/diag\_scripts/your\_diagnostic/your\_script.py

In addition to prospector, we also use flake8 to automatically check for obvious bugs and formatting mistakes.

When you make a pull request, adherence to the Python development best practices is checked in two ways:

- 1. As part of the unit tests, flake8 is run by CircleCI, see the section on Tests for more information.
- 2. Codacy is a service that runs prospector (and other code quality tools) on changed files and reports the results. Click the 'Details' link behind the Codacy check entry and then click 'View more details on Codacy Production' to see the results of the static code analysis done by Codacy. If you need to log in, you can do so using your GitHub account.

A pull request should preferably not introduce any new prospector issues. However, we understand that there is a limit to how much time can be spent on polishing code, so up to 10 new (non-trivial) issues is still an acceptable amount. Formatting issues are considered trivial and need to be addressed. Note that the automatic code quality checks by prospector are really helpful to improve the quality of your code, but they are not flawless. If you suspect prospector or Codacy may be wrong, please ask the @ESMValGroup/tech-reviewers by commenting on your pull request.

Note that running prospector locally will give you quicker and sometimes more accurate results than waiting for Codacy.

Most formatting issues in Python code can be fixed automatically by running the commands

isort some\_file.py

to sort the imports in the standard way using isort and

yapf -i some\_file.py

to add/remove whitespace as required by the standard using yapf,

```
docformatter -i some_file.py
```

to run docformatter which helps formatting the docstrings (such as line length, spaces).

#### 30.4.2 NCL

Because there is no standard best practices document for NCL, we use PEP8 for NCL code as well, with some minor adjustments to accommodate for differences in the languages. The most important difference is that for NCL code the indentation should be 2 spaces instead of 4. Use the command nclcodestyle /path/to/file.ncl to check if your code follows the style guide. More information on the nclcodestyle command can be found *here*.

### 30.4.3 R

Best practices for R code are described in The tidyverse style guide. We check adherence to this style guide by using lintr on CircleCI. Please use styler to automatically format your code according to this style guide. In the future we would also like to make use of goodpractice to assess the quality of R code.

### 30.4.4 YAML

Please use yamllint to check that your YAML files do not contain mistakes. yamllint checks for valid syntax, common mistakes like key repetition and cosmetic problems such as line length, trailing spaces, wrong indentation, etc. When the tool complains about the maximum line length or too many spaces, please use your own best judgement about whether solving the issue will make your recipe more readable.

#### 30.4.5 Any text file

A generic tool to check for common spelling mistakes is codespell.

## **30.5 Documentation**

The documentation lives on docs.esmvaltool.org and is built using Sphinx. There are two main ways of adding documentation:

- 1. As written text in the directory doc/sphinx/source. When writing reStructuredText (.rst) files, please try to limit the line length to 80 characters and always start a sentence on a new line. This makes it easier to review changes to documentation on GitHub.
- 2. As docstrings or comments in code. For Python code, the docstrings of Python modules, classes, and functions that are mentioned in doc/sphinx/source/api are used to generate documentation. This results in the *ESMValTool Code API Documentation*.

### 30.5.1 What should be documented

#### See also Recipe and diagnostic documentation and Dataset documentation.

Any code documentation that is visible on docs.esmvaltool.org should be well written and adhere to the standards for documentation for the respective language. Note that there is no need to write extensive documentation for functions that are not visible in the online documentation. However, a short description in the docstring helps other contributors to understand what a function is intended to do and and what its capabilities are. For short functions, a one-line docstring is usually sufficient, but more complex functions might require slightly more extensive documentation.

### 30.5.2 How to build and view the documentation

Whenever you make a pull request or push new commits to an existing pull request, readthedocs will automatically build the documentation. The link to the documentation will be shown in the list of checks below your pull request, click 'Details' behind the check docs/readthedocs.org:esmvaltool to preview the documentation. If all checks were successful, you may need to click 'Show all checks' to see the individual checks.

To build the documentation on your own computer, go to the directory where the repository was cloned and run

sphinx-build doc/sphinx/source/ doc/sphinx/build/

or

sphinx-build -Ea doc/sphinx/source/ doc/sphinx/build/

to build it from scratch. Make sure that your newly added documentation builds without warnings or errors and looks correctly formatted. CircleCI will build the documentation with the command

#### sphinx-build -W doc/sphinx/source/ doc/sphinx/build/

to catch mistakes that can be detected automatically.

The configuration file for Sphinx is doc/sphinx/source/conf.py and the configuration file for ReadTheDocs is .readthedocs.yaml.

When reviewing a pull request, always check that the documentation checks shown below the pull request were successful. Successful checks have a green  $\checkmark$  in front, a means the test job failed.

#### 30.5.3 Integration with the ESMValCore documentation

The ESMValCore documentation is hosted as a subproject of the ESMValTool documentation on readthedocs. To link to a section from the ESMValCore documentation from the reStructuredText (.rst) files, use the usual :ref: but prefix the reference with esmvalcore:. For example, :ref:`esmvalcore:recipe` to link to The recipe format.

There is a script that generates the navigation menu shown on the left when you view the documentation. This script is called doc/sphinx/source/gensidebar.py in the ESMValTool repository and it should be identical to doc/gensidebar.py in the ESMValCore repository, or the sidebar will change when navigating from the ESMValTool documentation to the ESMValCore documentation and vice-versa.

## 30.6 Tests

To check various aspects of the recipes and code, there tests available in the tests directory.

Whenever you make a pull request or push new commits to an existing pull request, these tests will be run automatically on CircleCI. The results appear at the bottom of the pull request. Click on 'Details' for more information on a specific test job. To see some of the results on CircleCI, you may need to log in. You can do so using your GitHub account.

To run the tests on your own computer, go to the directory where the repository is cloned and run the command pytest.

Have a look at *Testing recipes* for information on testing recipes.

Every night, more extensive tests are run to make sure that problems with the installation of the tool are discovered by the development team before users encounter them. These nightly tests have been designed to mimic the installation procedures described in the documentation, e.g. in the *Installation* chapter. The nightly tests are run using both CircleCI and GitHub Actions, the result of the tests ran by CircleCI can be seen on the CircleCI project page and the result of the tests ran by GitHub Actions can be viewed on the Actions tab of the repository.

The configuration of the tests run by CircleCI can be found in the directory .circleci, while the configuration of the tests run by GitHub Actions can be found in the directory .github/workflows.

When reviewing a pull request, always check that all test jobs on CircleCI were successful. Successful test jobs have a green  $\checkmark$  in front, a means the test job failed.

# 30.7 List of authors

If you make a contribution to ESMValTool and you would like to be listed as an author (e.g. on Zenodo), please add your name to the list of authors in CITATION.cff and generate the entry for the .zenodo.json file by running the commands

```
pip install cffconvert
cffconvert --infile CITATION.cff --format zenodo --outfile .zenodo.json
```

Presently, this method unfortunately discards entries *communities* and *grants* from that file; please restore them manually.

Note that authors of recipes and/or diagnostics also need to be added to the file esmvaltool/config-references.yml, see *Recording provenance* for more information.

## **30.8 Dependencies**

Before considering adding a new dependency, carefully check that the license of the dependency you want to add and any of its dependencies are compatible with the Apache 2.0 license that applies to the ESMValTool. Note that GPL version 2 license is considered incompatible with the Apache 2.0 license, while the compatibility of GPL version 3 license with the Apache 2.0 license is questionable. See this statement by the authors of the Apache 2.0 license for more information.

When adding or removing dependencies, please consider applying the changes in the following files:

- environment.yml contains dependencies that cannot be installed from PyPI/Julia package registry
- environment\_osx.yml contains development dependencies for MacOSX. Should be the same as environment.yml, but currently without multi language support.
- esmvaltool/install/Julia/Project.toml contains Julia dependencies that can be installed from the default Julia package registry

• setup.py contains all Python dependencies, regardless of their installation source

Note that packages may have a different name on conda-forge than on PyPI or CRAN.

Several test jobs on CircleCI related to the installation of the tool will only run if you change the dependencies. These will be skipped for most pull requests.

When reviewing a pull request where dependencies are added or removed, always check that the changes have been applied in all relevant files.

# **30.9 Pull request checks**

To check that a pull request is up to standard, several automatic checks are run when you make a pull request. Read more about it in the *Tests* and *Documentation* sections. Successful checks have a green  $\checkmark$  in front, a means the check failed.

If you need help with the checks, please ask the technical reviewer of your pull request for help. Ask @ESMValGroup/tech-reviewers if you do not have a technical reviewer yet.

If the checks are broken because of something unrelated to the current pull request, please check if there is an open issue that reports the problem and create one if there is no issue yet. You can attract the attention of the @ESMValGroup/esmvaltool-coreteam by mentioning them in the issue if it looks like no-one is working on solving the problem yet. The issue needs to be fixed in a separate pull request first. After that has been merged into the main branch and all checks are green again on the main branch, merge it into your own branch to get the tests to pass.

When reviewing a pull request, always make sure that all checks were successful. If the Codacy check keeps failing, please run prospector locally. If necessary, ask the pull request author to do the same and to address the reported issues. See the section on *code\_quality* for more information. Never merge a pull request with failing CircleCI or readthedocs checks.

CHAPTER

## THIRTYONE

# MAKING A NEW DIAGNOSTIC OR RECIPE

## **31.1 Getting started**

Please discuss your idea for a new diagnostic or recipe with the development team before getting started, to avoid disappointment later. A good way to do this is to open an issue on GitHub. This is also a good way to get help.

# 31.2 Creating a recipe and diagnostic script(s)

First create a recipe in esmvaltool/recipes to define the input data your analysis script needs and optionally preprocessing and other settings. Also create a script in the esmvaltool/diag\_scripts directory and make sure it is referenced from your recipe. The easiest way to do this is probably to copy the example recipe and diagnostic script and adjust those to your needs.

If you have no preferred programming language yet, Python 3 is highly recommended, because it is most well supported. However, NCL, R, and Julia scripts are also supported.

Good example recipes for the different languages are:

- python: esmvaltool/recipes/examples/recipe\_python.yml
- R: esmvaltool/recipes/examples/recipe\_r.yml
- julia: esmvaltool/recipes/examples/recipe\_julia.yml
- ncl: esmvaltool/recipes/examples/recipe\_ncl.yml

Good example diagnostics are:

- python: esmvaltool/diag\_scripts/examples/diagnostic.py
- R: esmvaltool/diag\_scripts/examples/diagnostic.R
- julia: esmvaltool/diag\_scripts/examples/diagnostic.jl
- ncl: esmvaltool/diag\_scripts/examples/diagnostic.ncl

For an explanation of the recipe format, you might want to read about the ESMValTool recipe and have a look at the available preprocessor functions. For further inspiration, check out the already *available recipes and diagnostics*.

There is a directory esmvaltool/diag\_scripts/shared for code that is shared by many diagnostics. This directory contains code for creating common plot types, generating output file names, selecting input data, and other commonly needed functions. See *Shared diagnostic script code* for the documentation of the shared Python code.

# 31.3 Re-using existing code

Always make sure your code is or can be released under a license that is compatible with the Apache 2.0 license.

If you have existing code in a supported scripting language, you have two options for re-using it. If it is fairly mature and a large amount of code, the preferred way is to package and publish it on the official package repository for that language and add it as a dependency of ESMValTool. If it is just a few simple scripts or packaging is not possible (i.e. for NCL) you can simply copy and paste the source code into the esmvaltool/diag\_scripts directory.

If you have existing code in a compiled language like C, C++, or Fortran that you want to re-use, the recommended way to proceed is to add Python bindings and publish the package on PyPI so it can be installed as a Python dependency. You can then call the functions it provides using a Python diagnostic.

# 31.4 Recipe and diagnostic documentation

This section describes how to document a recipe. For more general information on writing documentation, see *Documentation*.

## 31.4.1 On readthedocs

Recipes should have a page in the Recipes chapter which describes what the recipe/diagnostic calculates.

When adding a completely new recipe, please start by copying doc/sphinx/source/recipes/recipe\_template.rst.template to a new file doc/sphinx/source/recipes/recipe\_<name of diagnostic>.rst and do not forget to add your recipe to the index.

Fill all sections from the template:

- Add a brief description of the method
- · Add references
- Document recipe options for the diagnostic scripts
- Fill in the list of variables required to run the recipe
- · Add example images

An example image for each type of plot produced by the recipe should be added to the documentation page to show the kind of output the recipe produces. The '.png' files can be stored in a subdirectory specific for the recipe under doc/sphinx/source/recipes/figures and linked from the recipe documentation page. A resolution of 150 dpi is recommended for these image files, as this is high enough for the images to look good on the documentation webpage, but not so high that the files become large.

## 31.4.2 In the recipe

Fill in the documentation section of the recipe as described in Recipe section: documentation and add a description to each diagnostic entry. Please note that the maintainer entry is per se not necessary to run a recipe, but mandatory for recipes within the ESMValTool repository (enforced by a unit test). If no maintainer is available, use the single entry unmaintained. When reviewing a recipe, check that these entries have been filled with descriptive content.

## 31.4.3 In the diagnostic scripts

Functions implementing scientific formula should contain comments with references to the source paper(s) and formula number(s).

When reviewing diagnostic code, check that formulas are implemented according to the referenced paper(s) and/or other resources and that the computed numbers look as expected from literature.

# 31.5 Diagnostic output

Typically, diagnostic scripts create plots, but any other output such as e.g. text files or tables is also possible. Figures should be saved in the plot\_dir, either in both .pdf and .png format (preferred), or respect the output\_file\_type specified in the User configuration file. Data should be saved in the work\_dir, preferably as a .nc (NetCDF) file, following the CF-Conventions as much as possible.

Have a look at the *example scripts* for how to access the value of work\_dir, plot\_dir, and output\_file\_type from the diagnostic script code. More information on the interface between ESMValCore and the diagnostic script is available here and the description of the *Output* may also help to understand this.

If a diagnostic script creates plots, it should save the data used to create those plots also to a NetCDF file. If at all possible, there will be one NetCDF file for each plot the diagnostic script creates. There are several reasons why it is useful to have the plotted data available in a NetCDF file:

- for interactive visualization of the recipe on a website
- for automated regression tests, e.g. checking that the numbers are still the same with newer versions of libraries

If the output data is prohibitively large, diagnostics authors can choose to implement a write\_netcdf: false diagnostic script option, so writing the NetCDF files can be disabled from the recipe.

When doing a scientific review, please check that the figures and data look as expected from the literature and that appropriate references have been added.

# **31.6 Recording provenance**

When ESMValCore (the esmvaltool command) runs a recipe, it will first find all data and run the default preprocessor steps plus any additional preprocessing steps defined in the recipe. Next it will run the diagnostic script defined in the recipe and finally it will store provenance information. Provenance information is stored in the W3C PROV XML format and provided that the provenance tree is small, also plotted in an SVG file for human inspection. In addition to provenance information, a caption is also added to the plots.

Provenance information from the recipe is automatically recorded by ESMValCore, whereas diagnostic scripts must include code specifically to record provenance. See below for documentation of provenance attributes that can be included in a recipe. When contributing a diagnostic, please make sure it records the provenance, and that no warnings related to provenance are generated when running the recipe. To allow the ESMValCore to keep track of provenance (e.g. which input files were used to create what plots by the diagnostic script), it needs the Information provided by the diagnostic script to ESMValCore.

**Note:** Provenance is recorded by the esmvaltool command provided by the ESMValCore package. No \*\_provenance.xml files will be generated when re-running just the diagnostic script with the command that is displayed on the screen during a recipe run, because that will only run the diagnostic script.

## 31.6.1 Provenance items provided by the recipe

Provenance tags can be added in several places in the recipe. The Recipe section: documentation section provides information about the entire recipe.

For each diagnostic in the recipe, ESMValCore supports the following additional information:

- realms a list of high-level modeling components
- themes a list of themes

Please see the (installed version of the) file esmvaltool/config-references.yml for all available information on each item.

#### 31.6.2 Provenance items provided by the diagnostic script

For each output file produced by the diagnostic script, ESMValCore supports the following additional information:

- ancestors a list of input files used to create the plot.
- caption a caption text for the plot

Note that the level of detail is limited, the only valid choices for ancestors are files produced by ancestor tasks.

It is also possible to add more information for the implemented diagnostics using the following items:

- authors a list of authors
- references a list of references, see Adding references below
- projects a list of projects
- domains a list of spatial coverage of the dataset
- plot\_types a list of plot types if the diagnostic created a plot, e.g. error bar
- statistics a list of types of the statistic, e.g. anomaly
- long\_names a list of long names of used variables, e.g. Air Temperature

Arbitrarily named other items are also supported.

Please see the (installed version of the) file esmvaltool/config-references.yml for all available information on each item, see References configuration file for an introduction. It is also possible to add custom provenance information by adding items to each category in this file. In this file, the information is written in the form

```
key:
    value: description
```

for example

```
plot_types:
    errorbar: error bar plot
```

To use these items, include them in the provenance record dictionary in the form key: [value] i.e. for the example above as 'plot\_types': ['errorbar'].

In order to communicate with the diagnostic script, two interfaces have been defined, which are described in the ESM-ValCore documentation. Note that for Python and NCL diagnostics much more convenient methods are available than directly reading and writing the interface files. For other languages these are not implemented (yet).

Depending on your preferred programming language for developing a diagnostic, see the instructions and examples below on how to add provenance information:

## 31.6.3 Recording provenance in a Python diagnostic script

Always use esmvaltool.diag\_scripts.shared.run\_diagnostic() at the end of your script:

```
if __name__ == '__main__':
    with run_diagnostic() as config:
        main(config)
```

Create a provenance\_record for each diagnostic file (i.e. image or data file) that the diagnostic script outputs. The provenance\_record is a dictionary of provenance items, for example:

```
provenance_record = {
    'ancestors': ancestor_files,
    'authors': [
        'andela_bouwe',
        'righi_mattia',
],
    'caption': caption,
    'domains': ['global'],
    'plot_types': ['zonal'],
    'references': [
        'acknow_project',
],
    'statistics': ['mean'],
}
```

To save a matplotlib figure, use the convenience function <code>esmvaltool.diag\_scripts.shared.save\_figure()</code>. Similarly, to save Iris cubes use <code>esmvaltool.diag\_scripts.shared.save\_data()</code>. Both of these functions take provenance\_record as an argument and log the provenance accordingly. Have a look at the example Python diagnostic in esmvaltool/diag\_scripts/examples/diagnostic.py for a complete example.

For any other files created, you will need to make use of a *esmvaltool.diag\_scripts.shared*. *ProvenanceLogger* to log provenance. Include the following code directly after the file is saved:

```
with ProvenanceLogger(cfg) as provenance_logger:
    provenance_logger.log(diagnostic_file, provenance_record)
```

The full path of a diagnostic\_file can be obtained using *esmvaltool.diag\_scripts.shared.* get\_diagnostic\_filename.

## 31.6.4 Recording provenance in an NCL diagnostic script

Always call the log\_provenance procedure after plotting from your NCL diag\_script:

For example:

```
log_provenance(ncdf_outfile, \
    map@outfile, \
    "Mean of variable: " + var0, \
    "mean", \
    "global", \
```

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```
"geo", \
(/"righi_mattia", "gottschaldt_klaus-dirk"/), \
(/"acknow_author"/), \
metadata_att_as_array(info0, "filename"))
```

Have a look at the example NCL diagnostic in esmvaltool/diag\_scripts/examples/diagnostic.ncl for a complete example.

#### 31.6.5 Recording provenance in a Julia diagnostic script

The provenance information is written in a diagnostic\_provenance.yml that will be located in run\_dir. For example a provenance\_record can be stored in a yaml file as:

```
provenance_file = string(run_dir, "/diagnostic_provenance.yml")
open(provenance_file, "w") do io
    JSON.print(io, provenance_records, 4)
end
```

The provenance\_records can be defined as a dictionary of provenance items. For example:

```
provenance_records = Dict()
provenance_record = Dict(
    "ancestors" => [input_file],
    "authors" => ["vonhardenberg_jost", "arnone_enrico"],
    "caption" => "Example diagnostic in Julia",
    "domains" => ["global"],
    "projects" => ["crescendo", "c3s-magic"],
    "references" => ["zhang11wcc"],
    "statistics" => ["other"],
)
provenance_records[output_file] = provenance_record
```

Have a look at the example Julia diagnostic in esmvaltool/diag\_scripts/examples/diagnostic.jl for a complete example.

#### 31.6.6 Recording provenance in an R diagnostic script

The provenance information is written in a diagnostic\_provenance.yml that will be located in run\_dir. For example a provenance\_record can be stored in a yaml file as:

```
provenance_file <- paste0(run_dir, "/", "diagnostic_provenance.yml")
write_yaml(provenance_records, provenance_file)</pre>
```

The provenance\_records can be defined as a list of provenance items. For example:

```
provenance_records <- list()</pre>
```

```
provenance_record <- list(
    ancestors = input_filenames,
    authors = list("hunter_alasdair", "perez-zanon_nuria"),</pre>
```

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```
caption = title,
projects = list("c3s-magic"),
statistics = list("other"),
)
```

provenance\_records[[output\_file]] <- provenance\_record</pre>

## 31.7 Adding references

Recipes and diagnostic scripts can include references. When a recipe is run, citation information is stored in BibTeX format. Follow the steps below to add a reference to a recipe (or a diagnostic):

- make a tag that is representative of the reference entry. For example, righi15gmd shows the last name of the first author, year and journal abbreviation.
- add the tag to the references section in the recipe (or the diagnostic script provenance, see *recording-provenance*).
- make a BibTeX file for the reference entry. There are some online tools to convert a doi to BibTeX format like https://doi2bib.org/
- rename the file to the tag, keep the .bibtex extension.
- add the file to the folder esmvaltool/references.

Note: the references section in config-references.yaml has been replaced by the folder esmvaltool/ references.

## 31.8 Testing recipes

To test a recipe, you can run it yourself on your local infrastructure or you can ask the @esmvalbot to run it for you. To request a run of recipe\_xyz.yml, write the following comment below a pull request:

@esmvalbot Please run recipe\_xyz.yml

Note that only members of the @ESMValGroup/esmvaltool-developmentteam can request runs. The memory of the @esmvalbot is limited to 16 GB and it only has access to data available at DKRZ.

When reviewing a pull request, at the very least check that a recipes runs without any modifications. For a more thorough check, you might want to try out different datasets or changing some settings if the diagnostic scripts support those. A simple *tool* is available for testing recipes with various settings.

## 31.9 Detailed checklist for reviews

This (non-exhaustive) checklist provides ideas for things to check when reviewing pull requests for new or updated recipes and/or diagnostic scripts.

## **31.9.1 Technical reviews**

#### **Documentation**

Check that the scientific documentation of the new diagnostic has been added to the user's guide:

- A file doc/sphinx/source/recipes/recipe\_<diagnostic>.rst exists
- New documentation is included in doc/sphinx/source/recipes/index.rst
- Documentation follows template doc/sphinx/source/recipes/recipe\_template.rst.template
- Description of configuration options
- Description of variables
- Valid image files
- Resolution of image files (~150 dpi is usually enough; file size should be kept small)

#### Recipe

Check yaml syntax (with yamllint) and that new recipe contains:

- Documentation: description, authors, maintainer, references, projects
- Provenance tags: themes, realms

#### **Diagnostic script**

Check that the new diagnostic script(s) meet(s) standards. This includes the following items:

- In-code documentation (comments, docstrings)
- Code quality (e.g. no hardcoded pathnames)
- No Codacy errors reported
- Re-use of existing functions whenever possible
- Provenance implemented

#### **Run recipe**

Make sure new diagnostic(s) is working by running the ESMValTool with the recipe.

#### **Check output of diagnostic**

After successfully running the new recipe, check that:

- NetCDF output has been written
- Output contains (some) valid values (e.g. not only nan or zeros)
- Provenance information has been written

#### **Check automated tests**

Check for errors reported by automated tests

- Codacy
- CircleCI
- Documentation build

#### 31.9.2 Scientific reviews

#### Documentation added to user's guide

Check that the scientific documentation of the new diagnostic in doc/sphinx/source/recipes/ recipe\_<diagnostic>.rst:

- Meets scientific documentation standard and
- Contains brief description of method
- Contains references
- Check for typos / broken text
- Documentation is complete and written in an understandable language
- References are complete

#### Recipe

Check that new recipe contains valid:

- Documentation: description, references
- Provenance tags: themes, realms

#### **Diagnostic script**

Check that the new diagnostic script(s) meet(s) scientific standards. This can include the following items:

- Clear and understandable in-code documentation including brief description of diagnostic
- References
- Method / equations match reference(s) given

#### **Run recipe**

Make sure new diagnostic(s) is working by running the ESMValTool.

#### Check output of diagnostic

After successfully running the new recipe, check that:

- Output contains (some) valid values (e.g. not only nan or zeros)
- If applicable, check plots and compare with corresponding plots in the paper(s) cited

CHAPTER THIRTYTWO

# ESMVALTOOL POLICY ON BACKWARD COMPATIBILITY

### 32.1 Motivation

Development of recipes or conducting project-related work may require a rather long period of time during which new versions of the ESMValTool might become available. For a good user experience and a seamless workflow, users and developers need to know before upgrading to a new version if and how their work might be affected (backward compatibility). This includes, for instance, information about changes to technical features such as syntax of recipes and configuration files, and interfaces of shared functions, but also changes that affect the results of an ESMValTool run, e.g. modification of algorithms or changes to the order of operators. It is therefore essential that users and developers have the best advice on how and when to upgrade to new versions.

While trying to minimise the impact of new code developments on users and developers by maintaining backward compatibility where possible, this cannot always be guaranteed. A very restrictive policy might delay the ESMValTool development and make it more complex for developers to contribute.

This document outlines the key principles of an updated ESMValTool policy on backward compatibility.

# 32.2 Definitions

**Release:** A numbered version of ESMValCore / ESMValTool that has been released to the community, e.g. 2.4.0. This policy relates only to backward compatibility of releases, not to interim revisions of the main branch. Release numbers are of the format x.y.z, where:

- x indicates a major release
- y indicates a minor release
- z indicates a patch release

**Backward-incompatible change:** A change in ESMValCore or ESMValTool that causes a recipe to no longer run successfully (a *breaking change*), or which results in scientifically significant changes in results (a *science change*).

Breaking change: A change which causes a previously working recipe to no longer run successfully.

**Science change:** A change that alters scientific results. We do not formally distinguish between trivial science changes (e.g. from changes in the order of calculations) and more significant changes that would affect interpretation, although the detail that we communicate will share any understanding that we have regarding expected impact.

**Benign third-party dependency changes:** A change over which we have no control, but which we believe will only have trivial technical impacts (such as a change in font). Such changes are outside of the scope of this policy, though we will communicate about those we are aware of.

**Developer of backward-incompatible change:** For the purpose of this policy, developer is the individual that is responsible for the pull request (PR) that is not backward compatible.

Recipe developer: Someone who is developing a recipe that is not (yet) integrated into the repository.

**Recipe user:** For the purpose of this policy, a *recipe user* is anyone who runs a recipe using a *release* of ESMValTool. In this context, someone can be both a *recipe developer* and a *recipe user*, but they perform different activities in each capacity.

**Recipe maintainer:** First contact point for *integrated recipes* in case of problems with that recipe (see also *Maintaining a recipe*).

**Integrated recipes:** Recipes that are contained within the main branch of the ESMValTool repository, and can therefore be updated by any developer in line with the above guidance. Note that the recipe can be updated by someone other than the original author.

**User recipes:** Recipes developed by any developer outside of the main branch of the repository (i.e. on a dev/feature branch or outside the repository completely), and therefore cannot be updated by anyone else.

### 32.3 Scope

The ESMValTool and ESMValCore policy on backward compatibility aims at balancing two competing needs: the occasional need of improvements or maintenance to break backward compatibility and the need for stability for existing users and developers. The following aspects are covered by this policy:

- · Key principles and approaches to backward compatibility
- Guidelines and requirements for developers of backward-incompatible changes
- Communication with users and developers about backward-incompatible changes

Not within the scope of this policy are:

- Versioning scheme of ESMValTool
- Breakage of recipes due to changes in input data or dependencies. This is covered by the broken recipe policy.

# 32.4 Expectations of developers, users & funders

Stakeholders and their expectations and aims:

Projects / Funders

- Aim to facilitate scientific discovery
- Expect deliverables, e.g. new features/recipes
- Expect reproducible results

#### Recipe users

- Expect the recipe to work
- Expect the recipe to be easy to run
- Expect reproducible results
- Expect easy installation of ESMValTool

Recipe developers

- Develop recipes
- Expect their recipe to keep working with every new release of ESMValCore

- Expect ESMValCore bugfixes and new features to become available quickly
- Expect reproducible results
- Expect easy installation of ESMValTool

Core developers and recipe maintainers

- Fix bugs
- Add ESMValCore features requested by recipe developers
- Try to accommodate ESMValCore features contributed to by recipe developers
- Maintain existing recipes
- · Add new recipes
- Try to help (other) recipe developers with contributing their recipe
- Try to make installation as easy as possible

There is a tension between making new features available and keeping everything as is. New features facilitate scientific discovery because they enable *recipe developers* to do new research (e.g. analyse more data, new data, or perform a different analysis). Ensuring that every recipe ever made works with every new feature is technically a lot of work, more than we have funding for. Therefore we need to make sure that new features are added regularly, but we respect the timescale on which *recipe developers* work when removing outdated features. Writing a paper and getting it published may take up to a year, so this seems a good timescale for larger changes. For changes that only affect a few users, shorter timescales could be acceptable. It is also good to note that we are part of a large software ecosystem (ESMValTool currently depends on over 500 different software packages), so we may not always be able to control at what pace changes are made to the software that we depend upon.

Two-way communication about new and removed features is needed to make this work. This requires active involvement from both the people developing the new features and the *recipe developers*. ESMValTool core developers and ESMValCore core developers need to make sure they clearly communicate changes. In the first place, this is done by writing good descriptions in issues and pull requests on GitHub, but some of this material also makes it to the changelog (where the GitHub pull requests are linked). It is highly recommended to communicate a relevant selection (e.g. important new, scheduled for removal, and removed features) also by other means, to ensure we reach as many people potentially affected as possible (see *Guidance on handling \*backward-incompatible changes*\* section below). We organize *monthly community* meetings where *recipe developers* can learn about the latest developments and everyone is welcome to join, ask questions, and provide feedback.

To meet the needs of users and funders, we should take reproducibility of older results seriously, but this should not hold us back from advancing our tools. We can support this by uploading a well tested container image to an archive that provides a DOI and by providing clear instructions on how to use such containers.

# 32.5 Helping developers to upgrade

*Recipe users* of ESMValTool should be able to successfully run *integrated recipes* using a *release*, since all *backward-incompatible changes* introduced between *releases* will have been fixed before the *release* is created. Please note the *broken recipe policy*.

However, *recipe developers* working on *user recipes* must be provided with information to enable them to adapt their code to resolve issues related to *backward-incompatible changes* when *backward-incompatible changes* are introduced to the main branch / when a *release* of ESMValTool is created.

#### 32.5.1 Guidance on handling backward-incompatible changes

As well as helping users to handle *backward-incompatible changes*, the policy and surrounding tools must help developers avoid making *backward-incompatible changes*. Not many ideas are developed on this yet, but components should include:

- Testing; *backward-incompatible changes* should be discovered as early in the development process as possible. This motivates continued investment in automated testing. To discover *backward-incompatible changes* early on in the development cycle, every night a selection of recipes is run on CircleCI. A recipe can be added to the test suite by adding it to the directory esmvaltool/recipes/testing. Only add recipes that require a small amount of data, i.e. considerably less than a gigabyte.
- Guidance on how to minimise the likelihood of introducing *backward-incompatible changes* and how to use deprecation warnings when needed (see developer guidance).
- *Instructions on how to provide text for the release notes* to assist *recipe developers* to adapt their recipe in light of the *backward-incompatible change*
- General instructions for *recipe developers* working on *user recipes* to enable them to adapt their code related to *backward-incompatible changes* (see ESMValTool\_Tutorial: issue #263).
- The developer or reviewer must tag the core development team to notify them of the *backward-incompatible change*, and give at least 2 weeks for objections to be raised before merging to the main branch. If a strong objection is raised the backward-incompatible change should not be merged until the objection is resolved.

### 32.5.2 Guidance on releasing backward-incompatible changes

During the *release* process, the following information must be provided:

- **Release notes:** The *release* notes are already documented in the *ESMValTool Changelog* and ESMValCore Changelog, and "*backward-incompatible changes*" is the first section after "Highlights".
  - backward-incompatible changes: This section must include clear instructions detailing how a *recipe developer* should adapt their code for each item in this section, whether the adapted code would introduce a *science change*, and the list of affected or fixed *integrated recipes* that had to be updated due to the *backward-incompatible changes*, if applicable (to provide further examples to *recipe developers* working on *user recipes* of how to adapt code).
  - Developer guidance: Developers of backward-incompatible changes must:
    - \* write and include the information required for the "*backward-incompatible changes*" section in the PR that introduces the *backward-incompatible change*
    - \* share details of the *backward-incompatible change* at the next monthly ESMValTool community meeting
  - Communication: The *release* notes must be shared with the community (for example, via the *User mailing list* and the Community repository) at the point the first *release* candidate is made, highlighting the *"backward-incompatible changes"* section. The User Engagement Team should organise the communication of new *releases* together with the *Release manager*.

# CHAPTER THIRTYTHREE

# **BROKEN RECIPE POLICY**

Recipes might stop working for different reasons. Among those are, for instance, withdrawal of datasets used by the recipe (i.e. the recipe contains data that are no longer publicly available), backward incompatible development of the ESMValTool including new features or retiring old ones as well as changes to Python or used dependencies such as library functions. In such cases, the *Maintaining a recipe* is contacted by the technical lead development team (@ESMValGroup/technical-lead-development-team) to find a solution, fixing the affected recipe and checking the scientific output after applying the fix. If no recipe maintainer is available, such recipes will be flagged by the release manager during the *Release schedule and procedure* as "broken". For this, the affected recipe will be added to the *list of broken recipes*, together with the version number of the last known release in which the recipe maintainer could be found during this time, the affected recipe and diagnostics will be retired. This means the recipe and diagnostic code are removed from the ESMValTool main branch by the release manager and thus will not be included in future releases. Only the scientific documentation of the recipe (and diagnostics) will be kept in the user and developer guide with an additional note and link to the last release in which the recipe was still fully functional.

CHAPTER

### THIRTYFOUR

### **MAKING A NEW DATASET**

If you are contributing a new dataset, please have a look at *Writing a CMORizer script for an additional dataset* for how to do so. Please always create separate pull requests for CMORizer scripts, even when introducing a new dataset or updating an existing dataset with a new recipe.

If you are updating a CMORizer script to support a different dataset version, please have a look at *Support for multiple versions of a dataset* for how to handle multiple dataset versions.

### 34.1 Dataset documentation

The documentation required for a CMORizer script is the following:

- Make sure that the new dataset is added to the list of *Supported datasets for which a CMORizer script is available* and to the file datasets.yml.
- The code documentation should contain clear instructions on how to obtain the data.
- A BibTeX file named <dataset>.bibtex defining the reference for the new dataset should be placed in the directory esmvaltool/references/, see *Adding references* for detailed instructions.

For more general information on writing documentation, see Documentation.

### 34.2 Testing

When contributing a new script, add an entry for the CMORized data to recipes/examples/recipe\_check\_obs.yml and run the recipe, to make sure the CMOR checks pass without warnings or errors.

To test a pull request for a new CMORizer script:

- 1. Download the data following the instructions included in the script and place it in the RAWOBS path specified in your config-user.yml
- 2. If available, use the downloading script by running esmvaltool data download --config\_file <config\_file> <dataset>
- 3. Run the cmorization by running esmvaltool data format <config-file> <dataset>
- 4. Copy the resulting data to the OBS (for CMIP5 compliant data) or OBS6 (for CMIP6 compliant data) path specified in your config-user.yml
- 5. Run recipes/examples/recipe\_check\_obs.yml with the new dataset to check that the data can be used

### 34.3 Scientific sanity check

When contributing a new dataset, we expect that the numbers and units of the dataset look physically meaningful. The scientific reviewer needs to check this.

### 34.4 Data availability

Once your pull request has been approved by the reviewers, ask a member of @OBS-maintainers to add the new dataset to the data pool at DKRZ and CEDA-Jasmin. This team is in charge of merging CMORizer pull requests.

### 34.5 Detailed checklist for reviews

This (non-exhaustive) checklist provides ideas for things to check when reviewing pull requests for new or updated CMORizer scripts.

#### 34.5.1 Dataset description

Check that new dataset has been added to the table of observations defined in the ESMValTool guide user's guide in section *Obtaining input data* (generated from doc/sphinx/source/input.rst). Check that the new dataset has also been added to the file datasets.yml.

#### 34.5.2 BibTeX info file

Check that a BibTeX file, i.e. <dataset>.bibtex defining the reference for the new dataset has been created in esmvaltool/references/.

#### 34.5.3 recipe\_check\_obs.yml

Check that new dataset has been added to the testing recipe esmvaltool/recipes/examples/recipe\_check\_obs.yml

#### 34.5.4 Downloader script

If present, check that the new downloader script esmvaltool/cmorizers/data/downloaders/datasets/ <dataset>.py meets standards. This includes the following items:

- Code quality checks
  - 1. Code quality
  - 2. No Codacy errors reported

#### 34.5.5 CMORizer script

Check that the new CMORizer script esmvaltool/cmorizers/data/formatters/datasets/<dataset>.{py, ncl} meets standards. This includes the following items:

- In-code documentation (header) contains
  - 1. Download instructions
  - 2. Reference(s)
- Code quality checks
  - 1. Code quality (e.g. no hardcoded pathnames)
  - 2. No Codacy errors reported

#### 34.5.6 Config file

If present, check config file <dataset>.yml in esmvaltool/cmorizers/data/cmor\_config/ for correctness. Use yamllint to check for syntax errors and common mistakes.

#### 34.5.7 Run downloader script

If available, make sure the downloader script is working by running esmvaltool data download --config\_file <config-file> <dataset>

#### 34.5.8 Run CMORizer

Make sure CMORizer is working by running esmvaltool data format --config\_file <config-file> <dataset>

#### 34.5.9 Check output of CMORizer

After successfully running the new CMORizer, check that:

- Output contains (some) valid values (e.g. not only nan or zeros)
- Metadata is defined properly

Run esmvaltool/recipes/examples/recipe\_check\_obs.yml for new dataset.

#### 34.5.10 RAW data

Contact the team in charge of ESMValTool data pool (@OBS-maintainers) and request to copy RAW data to RA-WOBS/Tier2 (Tier3).

### 34.5.11 CMORized data

Contact the team in charge of ESMValTool data pool (@OBS-maintainers) and request to

- Merge the pull request
- Copy CMORized dataset to OBS/Tier2 (Tier3)
- Set file access rights for new dataset

CHAPTER THIRTYFIVE

# SUPPORT FOR MULTIPLE VERSIONS OF A DATASET

If you plan to update a CMORizer script to support a newer version of an existing dataset, indicate in the issue or pull request if support for previous versions should be kept. If the dataset is used in recipes, please also indicate if the recipes should be updated with the newest dataset version.

# 35.1 Policy for dropping support for older dataset versions

Support for older versions should preferably be kept as long as the data are publicly available. This ensures reproducibility and eases comparison of results of recipes using this dataset.

Even when previous dataset versions are no longer available or data issues have been fixed in a newer dataset version, it is preferable to keep support for the previous version in addition to supporting the newer version. In such cases, it is recommended to ask the recipe maintainers of recipes using the older version of the dataset to update to the newer version if possible so that support for the old version can be dropped in the future.

# 35.2 Naming conventions

If the data structure is rather similar between versions, a single CMORizer script (e.g. woa.py) and config file (e.g. WOA.yml) should be favored to handle multiple versions and avoid code duplication. Version-dependent data fixes can be applied based on the version keys defined in the config file.

In some cases, it can be simpler to use different names for different dataset versions (e.g. GCP2018 and GCP2020). CMORizer scripts and config files should be named accordingly.

CHAPTER THIRTYSIX

# **REVIEW OF PULL REQUESTS**

In the ESMValTool community we use pull request reviews to ensure all code and documentation contributions are of good quality. An introduction to code reviews can be found in The Turing Way, including why code reviews are important and advice on how to have constructive reviews.

Most pull requests will need two reviews before they can be merged. First a technical review takes place and then a scientific review. Once both reviewers have approved a pull request, it can be merged. These three steps are described in more detail below. If a pull request contains only technical changes, e.g. a pull request that corrects some spelling errors in the documentation or a pull request that fixes some installation problem, a scientific review is not needed.

If you are a regular contributor, please try to review a bit more than two other pull requests for every pull request you create yourself, to make sure that each pull request gets the attention it deserves.

If a pull request contains backward-incompatible changes, the developer or reviewer must tag the @ESMValGroup/esmvaltool-coreteam team to notify them of the *backward-incompatible change*.

### 36.1 1. Technical review

Technical reviews are done by the technical review team. This team consists of regular contributors that have a strong interest and experience in software engineering.

Technical reviewers use the technical checklist from the pull request template to make sure the pull request follows the standards we would like to uphold as a community. The technical reviewer also keeps an eye on the design and checks that no major design changes are made without the approval from the technical lead development team. If needed, the technical reviewer can help with programming questions, design questions, and other technical issues.

The technical review team can be contacted by writing @ESMValGroup/tech-reviewers in a comment on an issue or pull request on GitHub.

### 36.2 2. Scientific review

Scientific reviews are done by the scientific review team. This team consists of contributors that have a strong interest and experience in climate science or related domains.

Scientific reviewers use the scientific checklist from the pull request template to make sure the pull request follows the standards we would like to uphold as a community.

The scientific review team can be contacted by writing @ESMValGroup/science-reviewers in a comment on an issue or pull request on GitHub.

# 36.3 3. Merge

Pull requests are merged by the @ESMValGroup/esmvaltool-coreteam. Specifically, pull requests containing a *CMORizer script* can only be merged by a member of @OBS-maintainers, who will then add the CMORized data to the OBS data pool at DKRZ and CEDA-Jasmin. The team member who does the merge first checks that both the technical and scientific reviewer approved the pull request and that the reviews were conducted thoroughly. He or she looks at the list of files that were changed in the pull request and checks that all relevant checkboxes from the checklist in the pull request template have been added and ticked. Finally, he or she checks that the *Pull request checks* passed and merges the pull request. The person doing the merge commit edits the merge commit message so it contains a concise and meaningful text.

Any issues that were solved by the pull request can be closed after merging. It is always a good idea to check with the author of an issue and ask if it is completely solved by the related pull request before closing the issue.

If a pull request contains *backward-incompatible changes*, the person in charge of merging must give the core development team at least 2 weeks for objections to be raised before merging to the main branch. If a strong objection is raised the backward-incompatible change should not be merged until the objection is resolved.

The core development team can be contacted by writing @ESMValGroup/esmvaltool-coreteam in a comment on an issue or pull request on GitHub.

# 36.4 Frequently asked questions

### 36.4.1 How do I request a review of my pull request?

If you know a suitable reviewer, e.g. because your pull request fixes an issue that they opened or they are otherwise interested in the work you are contributing, you can ask them for a review by clicking the cogwheel next to 'Reviewers' on the pull request 'Conversation' tab and clicking on that person. When changing code, it is a good idea to ask the original authors of that code for a review. An easy way to find out who previously worked on a particular piece of code is to use git blame. GitHub will also suggest reviewers based on who previously worked on the files changed in a pull request. All recipes contain a list of the recipe authors (and some of them in addition a list of recipe maintainers). It is a good idea to ask these people for a review.

If there is no obvious reviewer, you can attract the attention of the relevant team of reviewers by writing to @ESMValGroup/tech-reviewers or @ESMValGroup/science-reviewers in a comment on your pull request. You can also label your pull request with one of the labels looking for technical reviewer or looking for scientific reviewer, though asking people for a review directly is probably more effective.

### 36.4.2 How do I optimize for a fast review?

When authoring a pull request, please keep in mind that it is easier and faster to review a pull request that does not contain many changes. Try to add one new feature per pull request and change only a few files. For the ESMValTool repository, try to limit changes to a few hundred lines of code and new diagnostics to not much more than a thousand lines of code. For the ESMValCore repository, a pull request should ideally change no more than about a hundred lines of existing code, though adding more lines for unit tests and documentation is fine.

If you are a regular contributor, make sure you regularly review other people's pull requests, that way they will be more inclined to return the favor by reviewing your pull request.

### 36.4.3 How do I find a pull request to review?

Please pick pull requests to review yourself based on your interest or expertise. We try to be self organizing, so there is no central authority that will assign you to review anything. People may advertise that they are looking for a reviewer by applying the label looking for technical reviewer or looking for scientific reviewer. If someone knows you have expertise on a certain topic, they might request your review on a pull request though. If your review is requested, please try to respond within a few days if at all possible. If you do not have the time to review the pull request, notify the author and try to find a replacement reviewer.

#### 36.4.4 How do I actually do a review?

To do a review, go to the pull request on GitHub, the list of all pull requests is available here https://github.com/ ESMValGroup/ESMValCore/pulls for the ESMValCore and here https://github.com/ESMValGroup/ESMValTool/ pulls for the ESMValTool, click the pull request you would like to review.

The top comment should contain (a selection of) the checklist available in the pull request template. If it is not there, copy the relevant items from the pull request template. Which items from the checklist are relevant, depends on which files are changed in the pull request. To see which files have changed, click the tab 'Files changed'. Please make sure you are familiar with all items from the checklist by reading the content linked from *Checklist for pull requests* and check all items that are relevant. Checklists with some of the items to check are available: *recipe and diagnostic checklist* and *dataset checklist*.

In addition to the items from the checklist, good questions to start a review with are 'Do I understand why these changes improve the tool?' (if not, ask the author to improve the documentation contained in the pull request and/or the description of the pull request on GitHub) and 'What could possibly go wrong if I run this code?'.

To comment on specific lines of code or documentation, click the 'plus' icon next to a line of code and write your comment. When you are done reviewing, use the 'Review changes' button in the top right corner to comment on, request changes to, or approve the pull request.

### 36.4.5 What if the author and reviewer disagree?

When the author and the reviewer of a pull request have difficulty agreeing on what needs to be done before the pull request can be approved, it is usually both more pleasant and more efficient to schedule a meeting or co-working session, for example using Google meet or Jitsi meet.

When reviewing a pull request, try to refrain from making changes to the pull request yourself, unless the author specifically agrees to those changes, as this could potentially be perceived as offensive.

If talking about the pull requests in a meeting still does not resolve the disagreement, ask a member of the @ESMValGroup/esmvaltool-coreteam for their opinion and try to find a solution.

CHAPTER THIRTYSEVEN

### **MAINTAINING A RECIPE**

As development of the ESMValTool continues, new features may be added, old ones replaced or retired or the interface of library functions may change when updating to new versions. This or for example the withdrawal of datasets used by a recipe can result in an existing recipe to stop working. Such "broken" recipes might require some work to fix such problems and make the recipe fully functional again.

A first **contact point** for the technical lead development team (@ESMValGroup/technical-lead-development-team) in such cases is the recipe "maintainer". The recipe maintainer is then asked to check the affected recipe and if possible, fix the problems or work with the technical lead development team to find a solution. Ideally, a recipe maintainer is able to tell whether the results of a fixed recipe are scientifically valid and look as expected. Being a recipe maintainer consists of the following tasks:

- answering timely to requests from the technical lead development team, e.g. if a recipe is broken
- if needed, checking and trying to fix their recipe(s) / working with the technical lead development team (e.g. fixing a recipe might include updating the actual recipe, diagnostic code or documentation)
- if needed, checking the output of the fixed recipe for scientific validity (asking science lead development team for advice if needed)
- If needed, change the documentation to reflect that some differences from the original results might appear (for reproducibility reasons. e.g. some missing datasets in the fixed recipe produce slight differences in the results but do not modify the conclusions)
- informing the core development team when no longer available as maintainer

Ideally, a recipe maintainer is named when contributing a new recipe to the ESMValTool. Recipe maintainers are asked to inform the core development team (@ESMValGroup/esmvaltool-coreteam) when they are no longer able to act as maintainer or when they would like to step down from this duty for any reason. The core development team will then try to find a successor. If no recipe maintainer can be found, the *policy on unmaintained broken (non-working) recipes* might apply eventually leading to retirement of the affected recipe.

CHAPTER THIRTYEIGHT

# UPGRADING A NAMELIST (RECIPE) OR DIAGNOSTIC TO ESMVALTOOL V2

This guide summarizes the main steps to be taken in order to port an ESMValTool namelist (now called **recipe**) and the corresponding diagnostic(s) from v1.0 to v2.0, hereafter also referred as the "*old*" and the "*new version*", respectively. The new ESMValTool version is being developed in the public git branch main. An identical version of this branch is maintained in the private repository as well and kept synchronized on an hourly basis.

In the following, it is assumed that the user has successfully installed ESMValTool v2 and has a rough overview of its structure (see Technical Overview).

### 38.1 Create a github issue

Create an issue in the public repository to keep track of your work and inform other developers. See an example here. Use the following title for the issue: "PORTING <recipe> into v2.0". Do not forget to assign it to yourself.

### 38.2 Create your own branch

Create your own branch from main for each namelist (recipe) to be ported:

```
git checkout main
git pull
git checkout -b <recipe>
```

main contains only v2.0 under the ./esmvaltool/ directory.

### 38.3 Convert xml to yml

In ESMValTool v2.0, the namelist (now recipe) is written in yaml format (Yet Another Markup Language format). It may be useful to activate the yaml syntax highlighting for the editor in use. This improves the readability of the recipe file and facilitates the editing, especially concerning the indentations which are essential in this format (like in python). Instructions can be easily found online, for example for emacs and vim.

A xml2yml converter is available in esmvaltool/utils/xml2yml/, please refer to the corresponding README file for detailed instructions on how to use it.

Once the recipe is converted, a first attempt to run it can be done, possibly starting with a few datasets and one diagnostics and proceed gradually. The recipe file ./esmvaltool/recipes/recipe\_perfmetrics\_CMIP5.yml can be used as an example, as it covers most of the common cases.

Do not forget to also rewrite the recipe header in a documentation section using the yaml syntax and, if possible, to add themes and realms item to each diagnostic section. All keys and tags used for this part must be defined in . /esmvaltool/config-references.yml. See ./esmvaltool/recipes/recipe\_perfmetrics\_CMIP5.yml for an example.

# 38.4 Create a copy of the diag script in v2.0

The diagnostic script to be ported goes into the directory ./esmvaltool/diag\_script/. It is recommended to get a copy of the very last version of the script to be ported from the version1 branch (either in the public or in the private repository). Just create a local (offline) copy of this file from the repository and add it to ../esmvaltool/diag\_script/ as a new file.

Note that (in general) this is not necessary for plot scripts and for the libraries in ./esmvaltool/diag\_script/ncl/lib/, which have already been ported. Changes may however still be necessary, especially in the plot scripts which have not yet been fully tested with all diagnostics.

# 38.5 Check and apply renamings

The new ESMValTool version includes a completely revised interface, handling the communication between the python workflow and the (NCL) scripts. This required several variables and functions to be renamed or removed. These changes are listed in the following table and have to be applied to the diagnostic code before starting with testing.

Name in v1.0	Name in v2.0	Affected code
<pre>getenv("ESMValTool_wrk_dir")</pre>	<pre>config_user_info@work_dir</pre>	all .ncl scripts
getenv(ESMValTool_att)	diag_script_info@att or config_user_info@att	all .ncl scripts
xml	yml	all scripts
<pre>var_attr_ref(0)</pre>	variable_info@reference_dataset	all .ncl scripts
<pre>var_attr_ref(1)</pre>	variable_info@alternative_dataset	all .ncl scripts
models	<pre>input_file_info</pre>	all .ncl scripts
models@name	<pre>input_file_info@dataset</pre>	all .ncl scripts
verbosity	<pre>config_user_info@log_level</pre>	all .ncl scripts
isfilepresent_esmval	fileexists	all .ncl scripts
messaging.ncl	logging.ncl	all .ncl scripts
<pre>info_output(arg1, arg2, arg3)</pre>	log_info(arg1) if arg3=1	all .ncl scripts
<pre>info_output(arg1, arg2, arg3)</pre>	log_debug(arg1) if arg3>1	all .ncl scripts
verbosity =	remove this statement	all .ncl scripts
config_user_info@verbosity		
<pre>enter_msg(arg1, arg2, arg3)</pre>	<pre>enter_msg(arg1, arg2)</pre>	all .ncl scripts
<pre>leave_msg(arg1, arg2, arg3)</pre>	<pre>leave_msg(arg1, arg2)</pre>	all .ncl scripts
noop()	appropriate if-else statement	all .ncl scripts
nooperation()	appropriate if-else stsatement	all .ncl scripts
fullpaths	<pre>input_file_info@filename</pre>	all .ncl scripts
<pre>get_output_dir(arg1, arg2)</pre>	<pre>config_user_info@plot_dir</pre>	all .ncl scripts
get_work_dir	<pre>config_user_info@work_dir</pre>	all .ncl scripts
inlist(arg1, arg2)	any(arg1.eq.arg2)	all .ncl scripts
load interface_scripts/*.ncl	<pre>load \$diag_scripts//</pre>	all .ncl scripts
	interface_scripts/interface.ncl	
<varname>_info.tmp</varname>	<varname>_info.ncl in preproc dir</varname>	all .ncl scripts

continues on next page

Name in v1.0	Name in v2.0	Affected code
ncl.interface	<pre>settings.ncl in run_dir and interface_scripts/interface.ncl</pre>	all .ncl scripts
<pre>load diag_scripts/lib/ncl/</pre>	<pre>load \$diag_scripts/shared/</pre>	all .ncl scripts
<pre>load plot_scripts/ncl/</pre>	<pre>load \$diag_scripts/shared/plot/</pre>	all .ncl scripts
<pre>load diag_scripts/lib/ncl/rgb/</pre>	<pre>load \$diag_scripts/shared/plot/ rgb/</pre>	all .ncl scripts
<pre>load diag_scripts/lib/ncl/ styles/</pre>	<pre>load \$diag_scripts/shared/plot/ styles</pre>	all .ncl scripts
<pre>load diag_scripts/lib/ncl/ misc_function.ncl</pre>	<pre>load \$diag_scripts/shared/plot/ misc_function.ncl</pre>	all .ncl scripts
LW_CRE, SW_CRE	lwcre, swcre	some yml recipes
check_min_max_models	check_min_max_datasets	all .ncl scripts
<pre>get_ref_model_idx</pre>	get_ref_dataset_idx	all .ncl scripts
get_model_minus_ref	get_dataset_minus_ref	all .ncl scripts

Table	1 –	- continued	from	previous	page
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The following changes may also have to be considered:

- namelists are now called recipes and collected in esmvaltool/recipes;
- models are now called datasets and all files have been updated accordingly, including NCL functions (see table above);
- run\_dir (previous interface\_data), plot\_dir, work\_dir are now unique to each diagnostic script, so it is no longer necessary to define specific paths in the diagnostic scripts to prevent file collision;
- input\_file\_info is now a list of a list of logicals, where each element describes one dataset and one variable. Convenience functions to extract the required elements (e.g., all datasets of a given variable) are provided in esmvaltool/interface\_scripts/interface.ncl;
- the interface functions interface\_get\_\* and get\_figure\_filename are no longer available: their functionalities can be easily reproduced using the input\_file\_info and the convenience functions in esmvaltool/ interface\_scripts/interface.ncl to access the required attributes;
- there are now only 4 log levels (debug, info, warning, and error) instead of (infinite) numerical values in verbosity
- diagnostic scripts are now organized in subdirectories in esmvaltool/diag\_scripts/: all scripts belonging to the same diagnostics are to be collected in a single subdirectory (see esmvaltool/diag\_scripts/ perfmetrics/ for example). This applies also to the aux\_ scripts, unless they are shared among multiple diagnostics (in this case they go in shared/);
- the relevant input\_file\_info items required by a plot routine should be passed as argument to the routine itself;
- upper case characters have to be avoided in script names, if possible.

As for the recipe, the diagnostic script ./esmvaltool/diag\_scripts/perfmetrics/main.ncl can be followed as working example.

# 38.6 Move preprocessing from the diagnostic script to the backend

Many operations previously performed by the diagnostic scripts, are now included in the backend, including level extraction, regridding, masking, and multi-model statistics. If the diagnostics to be ported contains code performing any of such operations, the corresponding code has to be removed from the diagnostic script and the respective backend functionality can be used instead.

The backend operations are fully controlled by the preprocessors section in the recipe. Here, a number of preprocessor sets can be defined, with different options for each of the operations. The sets defined in this section are applied in the diagnostics section to preprocess a given variable.

It is recommended to proceed step by step, porting and testing each operation separately before proceeding with the next one. A useful setting in the user configuration file (config-private.yml) called write\_intermediary\_cube allows writing out the variable field after each preprocessing step, thus facilitating the comparison with the old version (e.g., after CMORization, level selection, after regridding, etc.). The CMORization step of the new backend exactly corresponds to the operation performed by the old backend (and stored in the climo directory, now called preprec): this is the very first step to be checked, by simply comparing the intermediary file produced by the new backend after CMORization with the output of the old backend in the climo directory (see "Testing" below for instructions).

The new backend also performs variable derivation, replacing the calculate function in the variable\_defs scripts. If the recipe which is being ported makes use of derived variables, the corresponding calculation must be ported from the ./variable\_defs/<variable>.ncl file to ./esmvaltool/preprocessor/\_derive.py.

Note that the Python library esmval\_lib, containing the ESMValProject class is no longer available in version 2. Most functionalities have been moved to the new preprocessor. If you miss a feature, please open an issue on github [https://github.com/ESMValGroup/ESMValTool/issues].

# 38.7 Move diagnostic- and variable-specific settings to the recipe

In the new version, all settings are centralized in the recipe, completely replacing the diagnostic-specific settings in ./nml/cfg\_files/ (passed as diag\_script\_info to the diagnostic scripts) and the variable-specific settings in variable\_defs/<variable>.ncl (passed as variable\_info). There is also no distinction anymore between diagnostic- and variable-specific settings: they are collectively defined in the scripts dictionary of each diagnostic in the recipe and passed as diag\_script\_info attributes by the new ESMValTool interface. Note that the variable\_info logical still exists, but it is used to pass variable information as given in the corresponding dictionary of the recipe.

# 38.8 Make sure the diagnostic script writes NetCDF output

Each diagnostic script is required to write the output of the anaylsis in one or more NetCDF files. This is to give the user the possibility to further look into the results, besides the plots, but (most importantly) for tagging purposes when publishing the data in a report and/or on a website.

For each of the plot produced by the diagnostic script a single NetCDF file has to be generated. The variable saved in this file should also contain all the necessary metadata that documents the plot (dataset names, units, statistical methods, etc.). The files have to be saved in the work directory (defined in *cfg['work\_dir']* and *config\_user\_info@work\_dir*, for the python and NCL diagnostics, respectively).

### 38.9 Test the recipe/diagnostic in the new version

Once complete, the porting of the diagnostic script can be tested. Most of the diagnostic script allows writing the output in a NetCDF file before calling the plotting routine. This output can be used to check whether the results of v1.0 are correctly reproduced. As a reference for v1.0, it is recommended to use the development branch.

There are two methods for comparing NetCDF files: cdo and ncdiff. The first method is applied with the command:

cdo diffv old\_output.nc new\_output.nc

which will print a log on the stdout, reporting how many records of the file differ and the absolute/relative differences.

The second method produces a NetCDF file (e.g., diff.nc) with the difference between two given files:

ncdiff old\_output.nc new\_output.nc diff.nc

This file can be opened with ncview to visually inspect the differences.

In general, binary identical results cannot be expected, due to the use of different languages and algorithms in the two versions, especially for complex operations such as regridding. However, difference within machine precision are desirable. At this stage, it is essential to test all datasets in the recipe and not just a subset of them.

It is also recommended to compare the graphical output (this may be necessary if the ported diagnostic does not produce a NetCDF output). For this comparison, the PostScript format is preferable, since it is easy to directly compare two PostScript files with the standard diff command in Linux:

```
diff old_graphic.ps new_graphic.ps
```

but it is very unlikely to produce no differences, therefore visual inspection of the output may also be required.

### 38.10 Clean the code

Before submitting a pull request, the code should be cleaned to adhere to the coding standard, which are somehow stricter in v2.0. This check is performed automatically on GitHub (CircleCI and Codacy) when opening a pull request on the public repository. A code-style checker (nclcodestyle) is available in the tool to check NCL scripts and installed alongside the tool itself. When checking NCL code style, the following should be considered in addition to the warning issued by the style checker:

- two-space instead of four-space indentation is now adopted for NCL as per NCL standard;
- load statements for NCL standard libraries should be removed: these are automatically loaded since NCL v6.4.0 (see NCL documentation);
- the description of diagnostic- and variable-specific settings can be moved from the header of the diagnostic script to the recipe, since the settings are now defined there (see above);
- NCL print and printVarSummary statements must be avoided and replaced by the log\_info and log\_debug functions;
- for error and warning statements, the error\_msg function can be used, which automatically include an exit statement.

# 38.11 Update the documentation

If necessary, add or update the documentation for your recipes in the corrsponding rst file, which is now in doc\sphinx\source\recipes. Do not forget to also add the documentation file to the list in doc\sphinx\source\ annex\_c to make sure it actually appears in the documentation.

# 38.12 Open a pull request

Create a pull request on github to merge your branch back to main, provide a short description of what has been done and nominate one or more reviewers.

# CHAPTER THIRTYNINE

### **GITHUB WORKFLOW**

### 39.1 Basics

The source code of the ESMValTool is hosted on GitHub. The following description gives an overview of the typical workflow and usage for implementing new diagnostics or technical changes into the ESMValTool. For general information on Git, see e.g. the online documentation at https://www.git-scm.com/doc.

There are *two* ESMValTool GitHub repositories available:

- The PUBLIC GitHub repository is open to the public. The ESMValTool is released as open-source software under the Apache License 2.0. Use of the software constitutes acceptance of this license and terms. The PUBLIC ESMValTool repository is located at https://github.com/ESMValGroup/ESMValTool
- 2. The PRIVATE GitHub repository is restricted to the ESMValTool Development Team. This repository is only accessible to ESMValTool developers that have accepted the terms of use for the ESMValTool development environment. The use of the ESMValTool software and access to the private ESMValTool GitHub repository constitutes acceptance of these terms. When you fork or copy this repository, you must ensure that you do not copy the PRIVATE repository into an open domain! The PRIVATE ESMValTool repository for the ESMValTool development team is located at https://github.com/ESMValGroup/ESMValTool-private

All developments can be made in either of the two repositories. The creation of *FEATURE BRANCHES* (see below), however, is restricted to registered ESMValTool developers in both repositories. We encourage all developers to join the ESMValTool development team. Please contact the *ESMValTool Core Development Team* if you want to join the ESMValTool development team. The PRIVATE GitHub repository offers a central protected environment for ESM-ValTool developers who would like to keep their contributions undisclosed (e.g., unpublished scientific work, work in progress by PhD students) while at the same time benefiting from the possibilities of collaborating with other ESM-ValTool developers and having a backup of their work. *FEATURE BRANCHES* created in the PRIVATE repository are only visible to the ESMValTool development team but not to the public. The concept of a PRIVATE repository has proven to be very useful to efficiently share code during the development across institutions and projects in a common repository without having the contributions immediately accessible to the public.

Both, the PUBLIC and the PRIVATE repository, contain the following kinds of branches:

- MAIN BRANCH (official releases),
- DEVELOPMENT BRANCH (includes approved new contributions but version is not yet fully tested),
- *FEATURE BRANCH* (development branches for new features and diagnostics created by developers, the naming convention for *FEATURE BRANCHES* is <Project>\_<myfeature>).

# 39.2 Access rights

- Write access to the *MAIN* and *DEVELOPMENT BRANCH* in both, the PUBLIC and the PRIVATE GitHub repositories, is restricted to the *ESMValTool Core Development Team*.
- *FEATURE BRANCHES* in both the PUBLIC and the PRIVATE repository can be created by all members of the ESMValTool development team (i.e. members in the GitHub organization "ESMValGroup"). If needed, branches can be individually write-protected within each repository so that other developers cannot accidently push changes to these branches.

The *MAIN BRANCH* of the PRIVATE repository will be regularly synchronized with the *MAIN BRANCH* of the PUB-LIC repository (currently by hand). This ensures that they are identical at all times (see schematic in Figure Fig. 1). The recommended workflow for members of the ESMValTool development team is to create additional *FEATURE BRANCHES* in either the PUBLIC or the PRIVATE repository, see further instructions below.

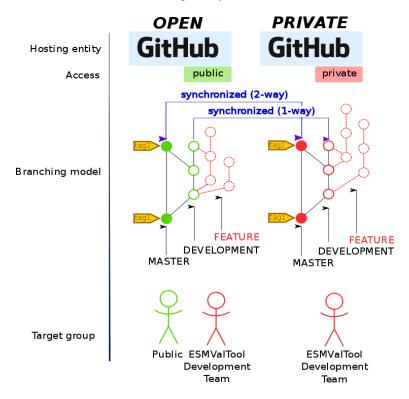


Fig. 1: Schematic diagram of the ESMValTool GitHub repositories.

# 39.3 Workflow

The following description gives an overview of the typical workflow and usage for implementing new diagnostics or technical changes into the ESMValTool. The description assumes that your local development machine is running a Unix-like operating system. For a general introduction to Git tutorials such as, for instance, https://www.git-scm.com/ docs/gittutorial are recommended.

#### 39.3.1 Getting started

First make sure that you have Git installed on your development machine. On shared machines, software is usually installed using the environment modules. Try e.g.

module avail git

if this is the case. You can ask your system administrator for assistance. You can test this with the command:

git --version

In order to properly identify your contributions to the ESMValTool you need to configure your local Git with some personal data. This can be done with the following commands:

```
git config --global user.name "YOUR NAME"
git config --global user.email "YOUR EMAIL"
```

Note: For working on GitHub you need to create an account and login to https://github.com/.

#### 39.3.2 Working with the ESMValTool GitHub Repositories

As a member of the ESMValTool development team you can create *FEATURE BRANCHES* in the PUBLIC as well as in the PRIVATE repository. We encourage all ESMValTool developers to use the following workflow for long-lived developments (>2 weeks).

- Login to GitHub.com
- On GitHub, go to the website of the ESMValTool repository (https://github.com/ESMValGroup/ ESMValTool-private or https://github.com/ESMValGroup/ESMValTool)
- Click on the button create FEATURE BRANCH
- Select the "DEVELOPMENT" BRANCH and create a new FEATURE BRANCH for the diagnostic/feature you want to implement. Please follow the following naming convention for your new FEATURE BRANCH: <Project>\_<myfeature>.

Branch: dev	elopment 🕶	New pull request	
Switch branches/tags			$\times$
Branches	Tags		
✓ development			
master			

- · Click the button "Clone or Download" and copy the URL shown there
- Open a terminal window and go to the folder where you would like to store your local copy of the ESMValTool source
- Type git clone, and paste the URL:

#### git clone <URL\_FROM\_CLIPBOARD>

This will clone the ESMValTool repository at GitHub to a local folder. You can now query the status of your local working copy with:

git status

You will see that you are on a branch called main and your local working copy is up to date with the remote repository. With

git branch --all

you can list all available remote and local branches. Now switch to your feature branch by:

```
git checkout <NAME_OF_YOUR_FEATURE_BRANCH>
```

You can now start coding. To check your current developments you can use the command

git status

You can add new files and folders that you want to have tracked by Git using:

git add <NEW\_FILE|FOLDER>

Commit your tracked changes to your local working copy via:

git commit -m "YOUR COMMIT MESSAGE"

You can inspect your changes with (use man git-log for all options):

git log

To share your work and to have an online backup, push your local development to your FEATURE BRANCH on GitHub:

git push origin <YOUR\_FEATURE\_BRANCH>

**Note:** An overview on Git commands and best practices can be found e.g. here: https://zeroturnaround.com/rebellabs/git-commands-and-best-practices-cheat-sheet/

#### 39.3.3 Pull requests

Once your development is completely finished, go to the GitHub website of the ESMValTool repository and switch to your *FEATURE BRANCH*. You can then initiate a pull request by clicking on the button "New pull request". Select the *DEVELOPMENT BRANCH* as "base branch" and click on "Create pull request". Your pull request will then be tested, discussed and implemented into the *DEVELOPMENT BRANCH* by the *ESMValTool Core Development Team*.

Attention: When creating a pull request, please carefully review the requirements and recommendations in CON-TRIBUTING.md and try to implement those (see also checklist in the pull request template). It is recommended that you create a draft pull request early in the development process, when it is still possible to implement feedback. Do not wait until shortly before the deadline of the project you are working on. If you are unsure how to implement any of the requirements, please do not hesitate to ask for help in the pull request.

### 39.3.4 GitHub issues

In case you encounter a bug of if you have a feature request or something similar you can open an issue on the PUBLIC ESMValTool GitHub repository.

# 39.4 General do-s and don't-s

#### 39.4.1 Do-s

- Create a *FEATURE BRANCH* and use exclusively this branch for developing the ESMValTool. The naming convention for *FEATURE BRANCHES* is <Project>\_<myfeature>.
- Comment your code as much as possible and in English.
- Use short but self-explanatory variable names (e.g., model\_input and reference\_input instead of xm and xr).
- Consider a modular/functional programming style. This often makes code easier to read and deletes intermediate variables immediately. If possible, separate diagnostic calculations from plotting routines.
- Consider reusing or extending existing code. General-purpose code can be found in esmval-tool/diag\_scripts/shared/.
- Comment all switches and parameters including a list of all possible settings/options in the header section of your code (see also ...).
- Use templates for recipes (see ...) and diagnostics (see ...) to help with proper documentation.
- Keep your FEATURE BRANCH regularly synchronized with the DEVELOPMENT BRANCH (git merge).
- Keep developments / modifications of the ESMValTool framework / backend / basic structure separate from developments of diagnostics by creating different *FEATURE BRANCHES* for these two kinds of developments. Create *FEATURE BRANCHES* for changes / modifications of the ESMValTool framework only in the *PUBLIC* repository.

### 39.4.2 Don't-s

- Do not use other programming languages than the ones currently supported (Python, R, NCL, Julia). If you are unsure what language to use, Python is probably the best choice, because it has very good libraries available and is supported by a large community. Contact the *ESMValTool Core Development Team* if you wish to use another language, but remember that only open-source languages are supported by the ESMValTool.
- Do not develop without proper version control (see do-s above).
- Avoid large (memory, disk space) intermediate results. Delete intermediate files/variables or see modular/functional programming style.
- Do not use hard-coded pathnames or filenames.
- Do not mix developments / modifications of the ESMValTool framework and developments / modifications of diagnostics in the same *FEATURE BRANCH*.

### MOVING WORK FROM THE PRIVATE TO THE PUBLIC REPOSITORY

In case you develop a new diagnostic with the ESMValTool, and you plan on publishing the results of the diagnostic in a peer-reviewed paper, you might want to develop the diagnostic in a slightly less open setting than the ESMValTool-public repository. That is what the ESMValTool-private repository is for. It would be great, though, if you would make the diagnostic available for the whole community after your paper was accepted. The steps that you need to take to develop a diagnostic in the private repository and then open a pull request for it in the public repository are described in the following:

### 40.1 1. Clone the private repository

For example, to clone a repository called esmvaltool-private, you would run:

```
git clone git@github.com:esmvalgroup/esmvaltool-private
```

or

git clone https://github.com/esmvalgroup/esmvaltool-private

### 40.2 2. Make a branch to develop your recipe and diagnostic

git checkout main git pull git checkout -b my-awesome-diagnostic

# 40.3 3. Develop your diagnostic in that branch and push it to the private repository

git push -u origin my-awesome-diagnostic the first time and git push any other time

# 40.4 4. Write and submit your paper

### 40.5 5. Push your branch to the public repository

Add the public repository as a remote git remote add public git@github.com:esmvalgroup/esmvaltool or git remote add public https://github.com/esmvalgroup/esmvaltool and push your branch to the public repository git push -u public my-awesome-diagnostic

# 40.6 6. Make a pull request in the public repository

Go to https://github.com/esmalgroup/esmvaltool/pulls and click the 'New pull request button'. Process reviewer comments and get it merged as described in *Review of pull requests*.

# 40.7 7. Obtain a DOI for your code and add it to your paper

Wait for a new release of ESMValTool. Releases are scheduled normally every four months. Find the release schedule here: *Release schedule*. With the next release, your diagnostic recipe and source code will automatically be included in the archive on Zenodo and you can add the DOI from Zenodo to your paper: https://zenodo.org/record/3698045

CHAPTER

### FORTYONE

# **RELEASE STRATEGY AND PROCEDURE**

These pages detail the release strategy and technical procedures during a release; these pages are very helpful if you are the next Release Manager.

For the release schdule, check the *Release schedule* to see upcoming and past releases.

# 41.1 Release schedule and procedure for ESMValCore and ESMVal-Tool

This document describes the process for the release of ESMValCore and ESMValTool. By following a defined process, we streamline the work, reduce uncertainty about required actions, and clarify the state of the code for the user.

ESMValTool follows a strategy of timed releases. That means that we do releases with a regular frequency and all features that are implemented up to a certain cut-off-point can go into the upcoming release; those that are not are deferred to the next release. This means that generally no release will be delayed due to a pending feature. Instead, the regular nature of the release guarantees that every feature can be released in a timely manner even if a specific target release is missed.

Because of limited resources, only the latest released versions of ESMValTool and ESMValCore is maintained. If your project requires longer maintenance or you have other concerns about the release strategy, please contact the ESMValTool core development team, see *Support*.

### 41.1.1 Overall Procedure

#### Timeline

- 1. Contributors assign issues (and pull requests) that they intend to finish before the due date, there is a separate milestone for ESMValCore and ESMValTool
- 2. The ESMValCore feature freeze takes place on the ESMValCore due date
- 3. Some additional testing of ESMValCore takes place
- 4. ESMValCore release
- 5. The ESMValTool feature freeze takes place
- 6. Some additional testing of ESMValTool takes place
- 7. ESMValTool release
- 8. Soon after the release, the core development team meets to coordinate the content of the milestone for the next release

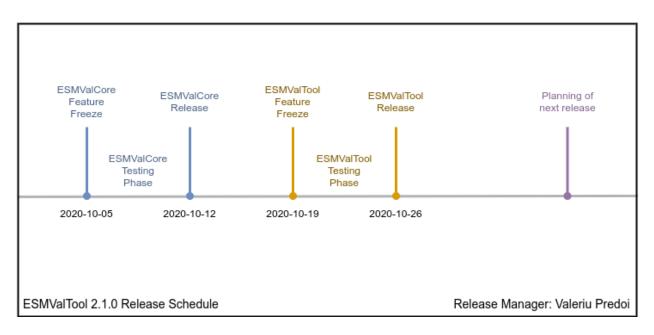


Fig. 1: Example of a Release Timeline (in this case for 2.1.0)

#### **Release schedule**

With the following release schedule, we strive to have three releases per year and to avoid releases too close to holidays, as well as avoiding weekends.

#### **Upcoming releases**

• 2.11.0 (Release Manager: Met Office: Emma Hogan, Chris Billows, Ed Gillett)

Planned	Done	Event	Changelog
2024-04-22		ESMValCore Feature Freeze	
2023-05-03		ESMValCore released	
2023-05-06		ESMValTool Feature Freeze	
2023-05-17		ESMValTool released	

#### **Past releases**

• 2.10.0 (Release Manager: Klaus Zimmermann)

Planned	Done	Event	Changelog
2023-10-02		ESMValCore Feature Freeze	
2023-10-09	2023-12-19	ESMValCore v2.10.0 released	v2.10.0
2023-10-16		ESMValTool Feature Freeze	
2023-10-16	2023-12-20	ESMValTool v2.10.0 released	v2.10.0

• 2.9.0 (Release Manager: Bouwe Andela)

Planned	Done	Event	Changelog
2023-06-05		ESMValCore Feature Freeze	
2023-06-12	2023-07-04	ESMValCore v2.9.0 released	v2.9.0
2023-06-19		ESMValTool Feature Freeze	
2023-06-26	2023-07-06	ESMValTool v2.9.0 released	v2.9.0

• 2.8.1 (Bugfix, Release Manager: Valeriu Predoi)

Done	Event	Changelog
2023-06-02	ESMValCore Release 2.8.1	v2.8.1

• 2.8.0 (Release Manager: Rémi Kazeroni)

Planned	Done	Event	Changelog
2023-03-03		ESMValCore Feature Freeze	
2023-03-20	2023-03-23	ESMValCore Release 2.8.0	v2.8.0
2023-03-17		ESMValTool Feature Freeze	
2023-03-27	2023-03-28	ESMValTool Release 2.8.0	v2.8.0

• 2.7.1 (Bugfix, Release Manager: Valeriu Predoi)

Done	Event	Changelog
2022-12-12	ESMValCore Release 2.7.1	v2.7.1

• 2.7.0 (Release Manager: Valeriu Predoi)

Planned	Done	Event	Changelog
2022-10-03		ESMValCore Feature Freeze	
2022-10-10	2022-10-13	ESMValCore Release 2.7.0	v2.7.0
2022-10-17		ESMValTool Feature Freeze	
2022-10-24	2022-10-28	ESMValTool Release 2.7.0	v2.7.0

• 2.6.0 (Release Manager: Saskia Loosveldt Tomas)

Planned	Done	Event	Changelog
2022-06-06		ESMValCore Feature Freeze	
2022-06-13	2022-07-15	ESMValCore Release 2.6.0	v2.6.0
2022-06-20		ESMValTool Feature Freeze	
2022-06-27	2022-07-25	ESMValTool Release 2.6.0	v2.6.0

• 2.5.0 (Coordinating Release Manager: Axel Lauer, team members: Manuel Schlund, Rémi Kazeroni)

Planned	Done	Event	Changelog
2022-02-07		ESMValCore Feature Freeze	
2022-02-14	2022-03-14	ESMValCore Release 2.5.0	v2.5.0
2022-02-21		ESMValTool Feature Freeze	
2022-02-28	2022-03-15	ESMValTool Release 2.5.0	v2.5.0

• 2.4.0 (Release Manager: Klaus Zimmermann)

Planned	Done	Event	Changelog
2021-10-04		ESMValCore Feature Freeze	
2021-10-11	2021-11-08	ESMValCore Release 2.4.0	v2.4.0
2021-10-18		ESMValTool Feature Freeze	
2021-10-25	2021-11-09	ESMValTool Release 2.4.0	v2.4.0

• 2.3.1 (Bugfix, Release Manager: Klaus Zimmermann)

Done	Event	Changelog
2021-07-23	ESMValCore Release 2.3.1	v2.3.1

• 2.3.0 (Release Manager: Klaus Zimmermann)

Planned	Done	Event	Changelog
2021-06-07		ESMValCore Feature Freeze	
2021-06-14	2021-06-14	ESMValCore Release 2.3.0	v2.3.0
2021-06-21		ESMValTool Feature Freeze	
2021-06-28	2021-07-27	ESMValTool Release 2.3.0	v2.3.0

• 2.2.0 (Release Manager: Javier Vegas-Regidor)

Planned	Done	Event	Changelog
2021-02-01		ESMValCore Feature Freeze	
2021-02-07	2021-02-09	ESMValCore Release 2.2.0	v2.2.0
2021-02-14		ESMValTool Feature Freeze	
2021-02-21	2021-02-25	ESMValTool Release 2.2.0	v2.2.0

• 2.1.1 (Bugfix, Release Manager: Valeriu Predoi)

Done	Event	Changelog
2020-12-01	ESMValTool Release 2.1.1	v2.1.1

• 2.1.0 (Release Manager: Valeriu Predoi)

Planned	Done	Event	Changelog
2020-10-05		ESMValCore Feature Freeze	
2020-10-12	2020-10-12	ESMValCore Release 2.1.0	v2.1.0
2020-10-19		ESMValTool Feature Freeze	
2020-10-26	2020-10-26	ESMValTool Release 2.1.0	v2.1.0

• 2.0.0 (Release Manager: Bouwe Andela)

Planned	Done	Event	Changelog
2020-07-01		ESMValCore Feature Freeze	
2020-07-20	2020-07-20	ESMValCore Release 2.0.0	v2.0.0
2020-07-22		ESMValTool Feature Freeze	
2020-08-03	2020-08-03	ESMValTool Release 2.0.0	v2.0.0

#### **Detailed timeline steps**

These are the detailed steps to take to make a release.

- 1. Populate the milestone
  - The core development team will make sure it adds issues that it intends to work on as early as possible.
  - Any contributor is welcome to add issues or pull requests that they intend to work on themselves to a milestone.
- 2. ESMValCore feature freeze, testing, and release candidates
  - A release branch is created and branch protection rules are set up so only the release manager (i.e. the person in charge of the release branch) can push commits to that branch.
  - Make a release candidate with the release branch following the ESMValCore release instructions.
  - Uncomment the release candidate channel item (i.e. conda-forge/label/esmvalcore\_rc) in the environment.yml of ESMValTool to add it to the list of channels used. Adjust the pin on ESMVal-Core after each release candidate (e.g. esmvalcore==2.8.0rc1). Check that the environment creation of ESMValTool works fine and contains the latest release candidate version.
  - Run all the recipes (optionally with a reduced amount of data) to check that they still work with the release candidate.
  - If a bug is discovered that needs to be fixed before the release, a pull request can be made to the main branch to fix the bug. The person making the pull request can then ask the release manager to cherry-pick that commit into the release branch.
  - Make another release candidate including the bugfix(es) and run the affected recipes again to check for further bugs.
  - Make as many release candidates for ESMValCore as needed in order to fix all the detected bugs.
- 3. ESMValTool feature freeze
  - A release branch is created and branch protection rules are set up so only the release manager (i.e. the person in charge of the release branch) can push commits to that branch.
  - The creation of the release branch is announced to the ESMValTool development team along with the procedures to use the branch for testing and making last-minute changes (see next step).
- 4. Some additional testing of ESMValTool
  - Run all the recipes to check that they still work and generate the overview HTML pages.
  - Upload the results to the webpage at https://esmvaltool.dkrz.de/shared/esmvaltool/.
  - Compare the results to those obtained with the previous release.
  - Create a GitHub discussion to communicate about the results.
  - If there are differences with the previous release, ask recipe maintainers or authors to review the plots and NetCDF files of their diagnostics, for example by mentioning them in the discussion.

- If a bug is discovered that needs to be fixed before the release, a pull request can be made to the main branch to fix the bug. The person making the pull request can then ask the release manager to cherry-pick that commit into the release branch.
- Update the *list of broken recipes* with new recipes that could not be run successfully during the testing. Open a separate GitHub issue for each failing recipe and assign the next milestone. Open an overview issue, see Issue #3484 for an example, and review past overview issues. Take action to ensure that the broken recipe policy is followed.
- 5. ESMValCore release
  - Make the official ESMValCore release with the last release candidate by following the ESMValCore release instructions.
- 6. ESMValTool release
  - Pin ESMValCore to the same version as ESMValTool in the environment.yml and on conda-forge. This way, we make sure that ESMValTool uses the ESMValCore version with which it has been tested. Make sure to comment again the release candidate channel once ESMValCore has been released.
  - Make the release by following *How to make an ESMValTool release*.
- 7. Announce the releases
  - Ask the user engagement team to announce the releases to the user mailing list, the development team mailing list, and on twitter.
- 8. Core development team meets to coordinate the content of next milestone
  - Create a doodle for the meeting or even better, have the meeting during an ESMValTool workshop
  - Prepare the meeting by filling the milestone
  - At the meeting, discuss
    - If the proposed issues cover everything we would like to accomplish
    - Are there things we need to change about the release process
    - Who will be the release manager(s) for the next release

## 41.1.2 Bugfix releases

Next to the feature releases described above, it is also possible to have bugfix releases (2.0.1, 2.0.2, etc). In general bugfix releases will only be done on the latest release, and may include ESMValCore, ESMValTool, or both.

### Procedure

- 1. One or more issues are resolved that are deemed (by the core development team) to warrant a bugfix release.
- 2. A release branch is created from the last release tag and the commit that fixes the bug/commits that fix the bugs are cherry-picked into it from the main branch.
- 3. Some additional testing of the release branch takes place.
- 4. The release takes place.

Compatibility between ESMValTool and ESMValCore is ensured by the appropriate version pinning of ESMValCore by ESMValTool.

## 41.1.3 Glossary

#### Feature freeze

The date on which no new features may be submitted for the upcoming release. After this date, only critical bug fixes can still be included to the *Release branch*. Development work can continue in the main branch. If you are unsure whether new developments could interfere with the release, check with the *Release manager*.

#### Milestone

A milestone is a list of issues and pull-request on GitHub. It has a due date, this date is the date of the feature freeze. Adding an issue or pull request indicates the intent to finish the work on this issue before the due date of the milestone. If the due date is missed, the issue can be included in the next milestone.

#### **Release manager**

The person in charge of making the release, both technically and organizationally. Appointed for a single release. Check the *Release schedule* to see who is the manager of the next release.

#### **Release branch**

The release branch can be used to do some additional testing before the release, while normal development work continues in the main branch. It will be branched off from the main branch after the feature freeze and will be used to make the release on the release date. The only way to still get something included in the release after the feature freeze is to ask the release manager to cherry-pick a commit from the main branch into this branch.

## 41.1.4 How to make an ESMValTool release

Before the actual release, a number of tests, and pre-release steps must be performed, a detailed workflow description can be found here *Release: recipes runs and comparison*.

The release manager makes the release, assisted by the release manager of the previous release, or if that person is not available, another previous release manager. Perform the steps listed below with two persons, to reduce the risk of error.

**Note:** The previous release manager ensures the current release manager has the required administrative permissions to make the release. Consider the following services: conda-forge, DockerHub, PyPI, and readthedocs.

The release of ESMValTool should come after the release of ESMValCore. To make a new release of the package, follow these steps:

#### 1. Check that all tests and builds work

- Check that the nightly test run on CircleCI was successful.
- Check that the GitHub Actions test runs were successful.
- Check that the documentation builds successfully on readthedocs.
- Check that the Docker images are building successfully.

All tests should pass before making a release (branch).

#### 2. Increase the version number

The version number is automatically generated from the information provided by git using setuptools-scm, but a static version number is stored in CITATION.cff. Make sure to update the version number and release date in CITATION.cff. See https://semver.org for more information on choosing a version number. Make sure that the ESMValCore version that is being used is set to the latest version. See the *dependencies* section in order to find more details on how update the ESMValCore version. Make a pull request and get it merged into main.

#### 3. Add release notes

Use the script *draft\_release\_notes.py* to create a draft of the release notes. This script uses the titles and labels of merged pull requests since the previous release. Open a discussion to allow members of the development team to nominate pull requests as highlights. Add the most voted pull requests as highlights at the beginning of changelog. After the highlights section, list any backward incompatible changes that the release may include. The *backward compatibility policy* lists the information that should be provided by the developer of any backward incompatible change. Make sure to also list any deprecations that the release may include, as well as a brief description on how to upgrade a deprecated feature. Review the results, and if anything needs changing, change it on GitHub and re-run the script until the changelog looks acceptable. Copy the result to the file doc/sphinx/source/changelog.rst. If possible, try to set the script dates to the date of the release you are managing. Make a pull request and get it merged into main.

#### 4. Create a release branch

Create a branch off the main branch and push it to GitHub. Ask someone with administrative permissions to set up branch protection rules for it so only you and the person helping you with the release can push to it. Announce the name of the branch in an issue and ask the members of the ESMValTool development team to run their favourite recipe using this branch.

#### 5. Make the release on GitHub

Do a final check that all tests on CircleCI and GitHub Actions completed successfully. Then click the releases tab and create the new release from the release branch (i.e. not from main). The release tag always starts with the letter v followed by the version number, e.g. v2.1.0.

#### 6. Merge the release branch back into the main branch

When the (pre-)release is tagged, it is time to merge the release branch back into *main*. We do this for two reasons, namely, one, to mark the point up to which commits in *main* have been considered for inclusion into the present release, and, two, to inform setuptools-scm about the version number so that it creates the correct version number in *main*. However, unlike in a normal merge, we do not want to integrate any of the changes from the release branch into main. This is because all changes that should be in both branches, i.e. bug fixes, originate from *main* anyway and the only other changes in the release branch relate to the release itself. To take this into account, we perform the merge in this case on the command line using the ours merge strategy (git merge -s ours), not to be confused with the ours option to the ort merge strategy (git merge -x ours). For details about merge strategies, see the above-linked page. To execute the merge use following sequence of steps

```
git fetch
git checkout main
git pull
git merge -s ours v2.1.x
git push
```

Note that the release branch remains intact and you should continue any work on the release on that branch.

#### 7. Create and upload the PyPI package

The package is automatically uploaded to the PyPI by a GitHub action. If has failed for some reason, build and upload the package manually by following the instructions below.

Follow these steps to create a new Python package:

- Check out the tag corresponding to the release, e.g. git checkout tags/v2.1.0
- Make sure your current working directory is clean by checking the output of git status and by running git clean -xdf to remove any files ignored by git.
- Install the required packages: python3 -m pip install --upgrade pep517 twine
- Build the package: python3 -m pep517.build --source --binary --out-dir dist/ . This command should generate two files in the dist directory, e.g. ESMValTool-2.1.0-py3-none-any.whl and ESMValTool-2.1.0.tar.gz.
- Upload the package: python3 -m twine upload dist/\* You will be prompted for an API token if you have not set this up before, see here for more information.

You can read more about this in Packaging Python Projects.

#### 8. Create the Conda package

The esmvaltool package is published on the conda-forge conda channel. This is done via a pull request on the esmvaltool-suite-feedstock repository.

After the upload of the PyPI package, this pull request is automatically opened by a bot. An example pull request can be found here. Follow the instructions by the bot to finalize the pull request. This step mostly contains updating dependencies that have been changed during the last release cycle. Once approved by the feedstock maintainers they will merge the pull request, which will in turn publish the package on conda-forge some time later. Contact the feedstock maintainers if you want to become a maintainer yourself.

#### 9. Check the Docker images

There are three main Docker container images available for ESMValTool on Dockerhub:

- esmvalgroup/esmvaltool:stable, built from docker/Dockerfile, this is a tag that is always the same as the latest released version. This image is only built by Dockerhub when a new release is created.
- esmvalgroup/esmvaltool:development, built from docker/Dockerfile.dev, this is a tag that always points to the latest development version of ESMValTool. This image is built by Dockerhub every time there is a new commit to the main branch on Github.
- esmvalgroup/esmvaltool:experimental, built from docker/Dockerfile.exp, this is a tag that always points to the latest development version of ESMValTool with the latest development version of ESMValCore. Note that some recipes may not work as expected with this image because the ESMValTool development version has been designed to work with the latest release of ESMValCore (i.e. not with the development version). This image is built by Dockerhub every time there is a new commit to the ESMValTool main branch on Github.

In addition to the three images mentioned above, there is an image available for every release (e.g. esmvalgroup/esmvaltool:v2.5.0). When working on the Docker images, always try to follow the best practices.

After making the release, check that the Docker image for that release has been built correctly by

- 1. checking that the version tag is available on Dockerhub and the stable tag has been updated,
- 2. running some recipes with the stable tag Docker container, for example one recipe for Python, NCL, R, and Julia,
- 3. running a recipe with a Singularity container built from the stable tag.

If there is a problem with the automatically built container image, you can fix the problem and build a new image locally. For example, to build and upload the container image for v2.5.0 of the tool run:

```
git checkout v2.5.0
git clean -x
docker build -t esmvalgroup/esmvaltool:v2.5.0 . -f docker/Dockerfile
docker push esmvalgroup/esmvaltool:v2.5.0
```

and if it is the latest release that you are updating, also run

```
docker tag esmvalgroup/esmvaltool:v2.5.0 esmvalgroup/esmvaltool:stable
docker push esmvalgroup/esmvaltool:stable
```

Note that the docker push command will overwrite the existing tags on Dockerhub.

If you would like to make a small change to an existing Docker container image, it is also possible to do just that using the docker commit command. Note that this is only recommended for very small changes, as it is not reproducible and it will add an extra layer, increasing the size of the image. To do this, start the container with docker run -it --entrypoint /bin/bash esmvalgroup/esmvaltool:v2.5.0 and make your changes. Exit the container by pressing *ctrl+d* and find it back by running docker ps -a. Find the *CONTAINER ID* of the image you would like to save and run docker commit -c 'ENTRYPOINT ["conda", "run", "--name", "esmvaltool", "esmvaltool"] ' 633696a8b53a esmvalgroup/esmvaltool:v2.5.0 where 633696a8b53c is the an example of a container ID, replace it by by the actual ID.

## 41.1.5 Changelog

- 2020-09-09 Converted to rst and added to repository (future changes tracked by git)
- 2020-09-03 Update during video conference (present: Bouwe Andela, Niels Drost, Javier Vegas, Valeriu Predoi, Klaus Zimmermann)
- 2020-07-27 Update including tidying up and Glossary by Klaus Zimmermann and Bouwe Andela
- 2020-07-23 Update to timeline format by Bouwe Andela and Klaus Zimmermann
- 2020-06-08 First draft by Klaus Zimmermann and Bouwe Andela

# 41.2 Release: recipes runs and comparison

The release procedure for ESMValTool is a fairly involved process (at the moment), so it is important to be very well organized and to have documented each procedural steps, so that the next release manager can follow said steps, and finalize the release without any delays.

The workflow below assumes an ESMValCore release candidate, or a completed stable release, have been released and deployed on conda-forge and PyPI; it also assumes the release manager has access to accounts on DKRZ/Levante.

Below is a list of steps that the release manager, together with the previous release manager, should go through before the actual release; these include testing the new code by running all available recipes in the main branch, and comparing the output against the previous release.

## 41.2.1 Open an issue on GitHub

First, open an issue on GitHub where the testing workflow before the release is documented (see example https://github. com/ESMValGroup/ESMValTool/issues/2881). Name it something relevant like "Recipe testing and comparison for release 2.x.x", and populate the issue description with information about where the testing is taking place, what tools are used, and what versions, here are some suggestions:

• path to the output directories on DKRZ/Levante

We should document various utilities' versions so that the work can be reproduced in case there is an issue, or release work needs to be picked up mid-release by another release manager:

• documenting conda/mamba versions:

```
mamba --version
```

• documenting git branch and its state:

#### git status

Furthermore, the runtime environment needs to be documented: make a copy of the environment file, and attach it in the release testing issue; to record the environment in a yaml file use e.g.

conda env export > ToolEnv\_v2xx\_Test.txt

Modifications to configuration files need to be documented as well. To test recipes, it is recommended to only use the default options and DKRZ data directories, simply by uncommenting the DKRZ-Levante block of a newly generated config-user.yml file.

### 41.2.2 Submit run scripts - test recipe runs

We are now ready to start running all the available recipes, to compare output against previous release. Running is currently done via batch scripts submitted to a schedulers (SLURM). Generate the submission scripts using the generate.py *utility Python script*.

You will have to set the name of your environment, your email address (if you want to get email notifications for successful/failed jobs) and the name of the directory you want to store the log files of the jobs. A compute project from which resources are billed needs to be set, and the default partition is set to *interactive*. More information on running jobs with SLURM on DKRZ/Levante can be found in the DKRZ documentation.

You can also specify the path to your config-user.yml file where max\_parallel\_tasks can be set. The script was found to work well with max\_parallel\_tasks=8. Some recipes need to be run with max\_parallel\_tasks=1 (large memory requirements, CMIP3 data, diagnostic issues, ...). These recipes are listed in ONE\_TASK\_RECIPES.

Some recipes need other job requirements, you can add their headers in the *SPECIAL\_RECIPES* dictionary. Otherwise the header will be written following the template that is written in the lines below. If you want to exclude recipes, you can do so by uncommenting the *exclude* lines.

Before submitting all jobs, it is recommended to try the batch script generation with submit = False and check the generated files. If recipes with special runtime requirements have been added to ESMValTool since the previous release, these may need to be added to *SPECIAL\_RECIPES* and/or to *ONE\_TASK\_RECIPES*. Other recipes should run successfully with the default SLURM settings set in this script.

The launch scripts will be saved in the same directory you execute the script from. These are named like launch\_recipe\_<name>.sh. To submit these scripts to the SLURM scheduler, use the sbatch launch\_recipe\_<name>.sh command. You can check the status of your BATCH queue by invoking:

squeue -u \$USER

Also, for computationally-heavy recipes, you can require more memory and/or time, see e.g. edited batch header below (note the *compute* partition which is used for such heavy runs):

```
#SBATCH --partition=compute
#SBATCH --time=08:00:00
#SBATCH --mem=0
#SBATCH --constraint=512G
```

**Note:** On DKRZ/Levante, a user can't have more than 20 SLURM jobs running at a time. As soon as a job is finished, the next one should start. More information on the job handling at DKRZ here. Also note that the --mem=0 argument needs be specified if any of the --constraint arguments are used for memory requests, so that the node's full memory is allocated.

### 41.2.3 Analyse the results

Once all jobs are completed, assemble some statistics so that issues with certain recipes can be followed-up, and document this information in the release issue, such as:

- number of successfully run recipes
- number of failed recipes with preprocessor errors (can they be fixed? Can the fixes be included in the release?)
- number of failed recipes with diagnostic errors (can they be fixed? Can the fixes be included in the release?)
- number of recipes that are missing data

• number of recipes that have various other issues (and document them)

To parse the output of all these runs, use the parse\_recipes\_output.py *utility Python script*. It is recommended to run the recipes with *log\_level: info* in your config file to enable the parsing script to run fast.

## 41.2.4 Share the results with the community

Create the debug.html and index.html overview webpages by running the *utility script* in the directory containing the recipe runs. These two files, together with the recipe output, need to be copied to the disk of a virtual machine (VM) used to display recipe output in webpages. Do not store final release results on the VM including /*preproc*/ dirs, the total size for all the recipes output, including /*preproc*/ dirs is in the 4.5TB ballpark, much too high for the VM storage capacity! Therefore, we would recommend using the option to remove preprocessing directories upon recipe running successfully --remove-preproc-dir=True at runtime, or set remove\_preproc\_dir: true in the configuration file.

Login and access to the DKRZ esmvaltool VM - results from recipe runs are stored on the VM; log in to the Levante head node and then continue to the VM with:

ssh user@esmvaltool.dkrz.de

where *user* is your DKRZ/Levante user name. Then create a new subdirectory in /shared/esmvaltool/ that will contain recipe output. This should be named like the ESMValCore version used for the testing, e.g. v2.x.xrcx or v2.x.x. Recipe output can be copied by doing from the VM:

By copying the debug.html and index.html files into /shared/esmvaltool/v2.x.x/, the output becomes available online, see for example. Before copying the recipe output to the VM, you may want to clean up your directory containing the results by removing any large preproc directories of failed runs and only keeping the last run for each recipe. This will help generating a clearer overview webpage. Note that the summarize.py script needs to be rerun if recipe runs were added or deleted from your testing directory.

Link the overview webpage to the release issue. This makes it much easier to ask for feedback from recipe developers and analyse failures.

Results produced with the final ESMValCore release candidate should be put in a VM directory named after the version number, e.g. v2.x.x. Once the release process is over, test results produced with previous release candidates can be deleted to save space on the VM.

**Note:** If you wrote recipe runs output to Levante's */scratch* partition, be aware that the data will be removed after two weeks, so you will have to quickly move the output data to the VM, using the nohup command above.

## 41.2.5 Running the comparison

To compare the newly produced output from running all recipes, follow these steps below.

Access to the DKRZ esmvaltool VM, then install miniconda on the VM, and if you have a Miniconda installer already downloaded in your Levante \$HOME

**Warning:** conda environments should not be created in the home directory because it is on a very small disk, but rather in a directory with your username under */mnt/esmvaltool\_disk2/work/<username>* 

Next, we need to set up the input files

The /work partition is visible from the VM so you can run the compare tool straight on the VM.

The steps to running the compare tool on the VM are the following:

- run date: log the run date here
- conda env: log the name of the conda environment you are using
- ESMValTool branch: log the name of the code branch you are using (e.g. v2.8.x)
- prerequisite install imagehash: pip install imagehash
- reference run (v2.7.0; previous stable release): export reference\_dir=/work/bd0854/b382109/v270 (contains preproc/ dirs too, 122 recipes)
- current run (v2.8.0): export current\_dir=path\_to\_current\_run
- run the *comparison script* with:

Copy the comparison txt file to the release issue. Some of the recipes will appear as having identical output to the one from previous release. However, others will need human inspection. Ask the recipe maintainers (@ESMValGroup/esmvaltool-recipe-maintainers) and ESMValTool Development Team (@ESMValGroup/esmvaltool-developmentteam) to provide assistance in checking the results. Here are some guidelines on how to perform the human inspection:

- look at plots from current run vs previous release run: most of them will be identical, but if Matplotlib has changed some plotting feature, images may look slightly different so the comparison script may report them if the difference is larger than the threshold but Mark I eyeball inspection will show they are identical
- other plots will differ due to changes in plot settings (different colours, axes etc) due to updated settings from the diagnostic developers: if they look similar enough, then it's fine
- report (and subsequently open issues) if you notice major differences in plots; most times a simple comment on the release issue, whereby you tag the diagnostic developers leads to them having a look at the plots and OK-ing them; if that's not the case, then open a separate issue. You can example of release issues containing overview lists and tables of failures and problems in 2881 and 3076.

## 41.2.6 Appendix

Here you can find a list of utility scripts used to run recipes and analyse the results:

- Python scripts that create slurm submission scripts and parse slurm log files.
- Python script that compares one or more recipe runs to known good previous run(s).
- Python script that creates the index.html and debug.html overview pages.

# Part IX

# Utilities

This section provides information on tools that are useful when developing ESMValTool. Tools that are specific to ESMValTool live in the esmvaltool/utils directory, while others can be installed using the usual package managers.

## FORTYTWO

## **PRE-COMMIT**

pre-commit is a handy tool that can run many tools for checking code quality with a single command. Usually it is used just before committing, to avoid accidentally committing mistakes. It knows knows which tool to run for each filetype, and therefore provides a convenient way to check your code!

To run pre-commit on your code, go to the ESMValTool directory (cd ESMValTool) and run

pre-commit run

By default, pre-commit will only run on the files that have been changed, meaning those that have been staged in git (i.e. after git add your\_script.py).

To make it only check some specific files, use

```
pre-commit run --files your_script.py
```

or

pre-commit run --files your\_script.R

Alternatively, you can configure pre-commit to run on the staged files before every commit (i.e. git commit), by installing it as a git hook using

pre-commit install

Pre-commit hooks are used to inspect the code that is about to be committed. The commit will be aborted if files are changed or if any issues are found that cannot be fixed automatically. Some issues cannot be fixed (easily), so to bypass the check, run

```
git commit --no-verify
```

or

git commit -n

or uninstall the pre-commit hook

pre-commit uninstall

Note that the configuration of pre-commit lives in .pre-commit-config.yaml.

# CHAPTER FORTYTHREE

# NCLCODESTYLE

A tool for checking the style of NCL code, based on pycodestyle. Install ESMValTool in development mode (pip install -e '.[develop]') to make it available. To use it, run

nclcodestyle /path/to/file.ncl

# FORTYFOUR

# **COLORMAP SAMPLES**

Tool to generate colormap samples for ESMValTool's default Python and NCL colormaps.

Run

esmvaltool colortables python

or

esmvaltool colortables ncl

to generate the samples.

CHAPTER FORTYFIVE

# **RUNNING MULTIPLE RECIPES**

It is possible to run more than one recipe in one go.

This can for example be achieved by using rose and/or cylc, tools that may be available at your local HPC cluster.

In the case in which neither rose nor cylc are available at your HPC cluster, it is possible to automatically generate job submission scripts, as well as a summary of the job outputs using the scripts available in esmvaltool/utils/batch-jobs.

# 45.1 Using cylc

A cylc suite for running all recipes is available in esmvaltool/utils/testing/regression. This suite is configured to work with versions of cylc older than 8.0.0.

To prepare for using this tool:

- 1. Log in to a system that uses slurm
- 2. Make sure the required CMIP and observational datasets are available and configured in config-user.yml
- 3. Make sure the required auxiliary data is available (see *recipe documentation*)
- 4. Install ESMValTool
- 5. Update config-user.yml so it points to the right data locations

Next, get started with cylc:

- 1. Run module load cylc
- Register the suite with cylc cylc register run-esmvaltool-recipes ~/ESMValTool/esmvaltool/ utils/testing/regression
- 3. Edit the suite if needed, this allows e.g. choosing which recipes will be run
- 4. Validate the suite cylc validate run-esmvaltool-recipes --verbose, this will e.g. list the recipes in the suite
- 5. Run all recipes cylc run run-esmvaltool-recipes
- 6. View progress cylc log run-esmvaltool-recipes, use e.g. cylc log run-all-esmvaltool-recipes examples-recipe\_python\_yml.1 --stdout to see the log of an individual esmvaltool run. Once the suite has finished running, you will see the message "WARNING suite stalled" in the log.
- 7. Stop the cylc run once everything is done cylc stop run-esmvaltool-recipes.

To generate an overview page of the recipe runs, use the summarize.py utility script.

# 45.2 Using Rose and cylc

It is possible to run more than one recipe in one go: currently this relies on the user having access to a HPC that has rose and cylc installed since the procedure involves installing and submitting a Rose suite. The utility that allows you to do this is esmvaltool/utils/rose-cylc/esmvt\_rose\_wrapper.py.

## 45.2.1 Base suite

The base suite to run esmvaltool via rose-cylc is u-bd684; you can find this suite in the Met Office Rose repository at:

https://code.metoffice.gov.uk/svn/roses-u/b/d/6/8/4/trunk/

When rose will be working with python3.x, this location will become default and the pipeline will access it independently of user, unless, of course the user will specify -s \$SUITE\_LOCATION; until then the user needs to grab a copy of it in \$HOME or specify the default location via -s option.

## 45.2.2 Environment

We will move to a unified and centrally-installed esmvaltool environment; until then, the user will have to alter the env\_setup script:

```
u-bd684/app/esmvaltool/env_setup
```

with the correct pointers to esmvaltool installation, if desired.

To be able to submit to cylc, you need to have the */metomi/* suite in path AND use a *python2.7* environment. Use the Jasmin-example below for guidance.

## 45.2.3 Jasmin-example

This shows how to interact with rose-cylc and run esmvaltool under cylc using this script:

```
export PATH=/apps/contrib/metomi/bin:$PATH
export PATH=/home/users/valeriu/miniconda2/bin:$PATH
mkdir esmvaltool_rose
cd esmvaltool_rose
cp ESMValTool/esmvaltool/utils/rose-cylc/esmvt_rose_wrapper.py .
svn checkout https://code.metoffice.gov.uk/svn/roses-u/b/d/6/8/4/trunk/ ~/u-bd684
[enter Met Office password]
[configure ~/u-bd684/rose_suite.conf]
[configure ~/u-bd684/rose_suite.conf]
[configure ~/u-bd684/app/esmvaltool/env_setup]
python esmvt_rose_wrapper.py -c config-user.yml \
-r recipe_autoassess_stratosphere.yml recipe_OceanPhysics.yml \
-d $HOME/esmvaltool_rose
rose suite-run u-bd684
```

Note that you need to pass FULL PATHS to cylc, no. or .. because all operations are done remotely on different nodes.

A practical actual example of running the tool can be found on JASMIN: /home/users/valeriu/esmvaltool\_rose. There you will find the run shell: run\_example, as well as an example how to set the configuration file. If you don't have Met Office credentials, a copy of *u-bd684* is always located in /home/users/valeriu/roses/u-bd684 on Jasmin.

# 45.3 Using the scripts in utils/batch-jobs

In utils/batch-jobs, you can find a script to generate slurm submission scripts for all available recipes in ESMValTool, as well as a script to parse the job outputs.

## 45.3.1 Using generate.py

The script generate.py, is a simple python script that creates slurm submission scripts, and if configured, submits them to the HPC cluster. It has been tested in DKRZ's Levante cluster.

The following parameters have to be set in the script in order to make it run:

- env, str: Name of the conda environment in which esmvaltool is installed.
- mail, *bool*: Whether or not to receive mail notifications when a submitted job fails or finishes successfully. Default is False.
- submit, *bool*: Whether or not to automatically submit the job after creating the launch script. Default value is False.
- account, str: Name of the DKRZ account in which the job will be billed.
- outputs, *str*: Name of the directory in which the job outputs (.out and .err files) are going to be saved. The outputs will be saved in */home/user/<outputs>*.
- conda\_path, str: Full path to the mambaforge/etc/profile.d/conda.sh executable.

Optionally, the following parameters can be edited:

- config\_file, str: Path to config-user.yml if default ~/.esmvaltool/config-user.yml not used.
- partition, *str*: Name of the DKRZ partition used to run jobs. Default is interactive to minimize computing cost compared to compute for which nodes cannot be shared.
- memory, *str*: Amount of memory requested for each run. Default is 64G to allow to run 4 recipes on the same node in parallel.
- time, *str*: Time limit. Default is 04:00:00 to increase the job priority. Jobs can run for up to 8 hours and 12 hours on the compute and interactive partitions, respectively.
- default\_max\_parallel\_tasks, *int*: Default is 8 which works for most recipes. For other cases, an entry needs to be made to the MAX\_PARALLEL\_TASKS dictionary (see below).

The script will generate a submission script for all recipes using by default the interactive queue and with a time limit of 4h. In case a recipe may require of additional resources, they can be defined in the SPECIAL\_RECIPES dictionary. The recipe name has to be given as a key in which the values are another dictionary. The latter are used to specify the partition in which to submit the recipe, the new time limit and other memory requirements given by the slurm flags --mem, --constraint or --ntasks. In general, an entry in SPECIAL\_RECIPES should be set as:

```
SPECIAL_RECIPES = {
    'recipe_name': {
        'partition': '#SBATCH --partition=<name_of_the_partition>',
        'time': '#SBATCH --time=<custom_time_limit>',
        'memory': '#SBATCH --mem=<custom_memory_requirement>' # --constraint or --nstasks_
        --can be used instead.
        },
}
```

Some recipes can only be run with a number of tasks less than default\_max\_parallel\_tasks for various reasons (memory issues, diagnostic issues, CMIP3 data used). These recipes need to be added to the MAX\_PARALLEL\_TASKS dictionary with a specific max\_parallel\_tasks value.

Note that the script has been optimized to use standard SLURM settings to run most recipes while minimizing the computational cost of the jobs and tailored runtime settings for resource-intensive recipes. It is only necessary to edit this script for recipes that have been added since the last release and cannot be run with the default settings.

In the case in which submit is set to True, but you want to exclude certain recipes from being submitted, their name can be added in the exclude list:

```
exclude = ['recipe_to_be_excluded_1', 'recipe_to_be_excluded_2']
```

## 45.3.2 Using parse\_recipes\_outputs

You can run this script (simply as a standalone Python script) after all recipes have been run, to gather a bird's eye view of the run status for each recipe; running the script provides you with a Markdown-formatted list of recipes that succeeded, recipes that failed due to a diagnostic error, and recipes that failed due to missing data (the two most common causes for recipe run failure). You should provide the location of the output log files from SLURM (\*.out and \*.err) to the script as well as a list of all available recipes. To generate the list, run the command:

for recipe in \$(esmvaltool recipes list | grep '\.yml\$'); do echo \$(basename "\$recipe");\_
\_done > all\_recipes.txt

To keep the script execution fast, it is recommended to use log\_level: info in your config-user.yml file so that SLURM output files are rather small.

# FORTYSIX

# **OVERVIEW OF RECIPE RUNS**

To create overview webpages of a set of recipe runs, run:

python esmvaltool/utils/testing/regression/summarize.py ~/esmvaltool\_output/

This will generate 2 html files:

- index.html that displays a summary of each recipe run, with a title and a representative plot, a short description of the aim of the recipe, and links to each individual run.
- debug.html that provides an overview table of successful and failed runs with links to each individual run, and computing resources used for each run.

## FORTYSEVEN

# **COMPARING RECIPE RUNS**

A command-line tool is available for comparing one or more recipe runs to known good previous run(s). This tool uses xarray to compare NetCDF files and difference hashing provided by imagehash to compare PNG images. All other file types are compared byte for byte.

To use it, first install the package imagehash:

pip install imagehash

Next, go to the location where ESMValTool is installed and run

where the first argument is a reference run or a directory containing such runs and the second and following arguments are directories with runs to compare to the reference run(s).

To compare all results from the current version to the previous version, use e.g.:

```
python esmvaltool/utils/testing/regression/compare.py /shared/esmvaltool/v2.4.0 /shared/

$\imple$ esmvaltool/v2.5.0
```

To get more information on how a result is different, run the tool with the --verbose flag.

CHAPTER FORTYEIGHT

# **TESTING RECIPE SETTINGS**

A tool for generating recipes with various diagnostic settings, to test of those work. Install ESMValTool in development mode (pip install -e '.[develop]') to make it available. To use it, run

test\_recipe --help

## FORTYNINE

# DRAFT\_RELEASE\_NOTES.PY

draft\_release\_notes.py is a script for drafting release notes based on the titles and labels of the GitHub pull requests that have been merged since the previous release.

To use it, install the package pygithub:

pip install pygithub

Create a GitHub access token (leave all boxes for additional permissions unchecked) and store it in the file  $\sim/.$  github\_api\_key.

Edit the script and update the date and time of the previous release and run the script:

python esmvaltool/utils/draft\_release\_notes.py \${REPOSITORY}

REPOSITORY can be either esmvalcore or esmvaltool depending on the release notes you want to create.

Review the resulting output (in .rst format) and if anything needs changing, change it on GitHub and re-run the script until the changelog looks acceptable. In particular, make sure that pull requests have the correct label, so they are listed in the correct category. Finally, copy and paste the generated content at the top of the changelog.

FIFTY

# **CONVERTING VERSION 1 NAMELISTS TO VERSION 2 RECIPES**

The xml2yml converter can turn the old xml namelists into new-style yml recipes. It is implemented as a xslt stylesheet that needs a processor that is xslt 2.0 capable. With this, you simply process your old namelist with the stylesheet xml2yml.xsl to produce a new yml recipe.

After the conversion you need to manually check the mip information in the variables! Also, check the caveats below!

## 50.1 Howto

One freely available processor is the Java based saxon. You can download the free he edition here. Unpack the zip file into a new directory. Then, provided you have Java installed, you can convert your namelist simply with:

java -jar \$SAXONDIR/saxon9he.jar -xsl:xml2yml.xsl -s:namelist.xml -o:recipe.yml

# 50.2 Caveats/Known Limitations

- At the moment, not all model schemes (OBS, CMIP5, CMIP5\_ETHZ...) are supported. They are, however, relatively easy to add, so if you need help adding a new one, please let me know!
- The documentation section (namelist\_summary in the old file) is not automatically converted.
- In version 1, one could name an exclude, similar to the reference model. This is no longer possible and the way to do it is to include the models with another additional\_models tag in the variable section. That conversion is not performed by this tool.

Authored by Klaus Zimmermann, direct questions and comments to klaus.zimmermann@smhi.se

# CHAPTER

# FIFTYONE

# **RECIPE FILLER**

If you need to fill in a blank recipe with additional datasets, you can do that with the command *recipe\_filler*. This runs a tool to obtain a set of additional datasets when given a blank recipe, and you can give an arbitrary number of data parameters. The blank recipe should contain, to the very least, a list of diagnostics, each with their variable(s). Example of running the tool:

```
recipe_filler recipe.yml
```

where *recipe.yml* is the recipe that needs to be filled with additional datasets; a minimal example of this recipe could be:

```
diagnostics:
    diagnostic:
    variables:
        ta:
        mip: Amon # required
        start_year: 1850 # required
        end_year: 1900 # required
```

# 51.1 Key features

- you can add as many variable parameters as are needed; if not added, the tool will use the "\*" wildcard and find all available combinations;
- you can restrict the number of datasets to be looked for with the dataset: key for each variable, pass a list of datasets as value, e.g. dataset: [MPI-ESM1-2-LR, MPI-ESM-LR];
- you can specify a pair of experiments, e.g. exp: [historical, rcp85] for each variable; this will look for each available dataset per experiment and assemble an aggregated data stretch from each experiment to complete for the total data length specified by start\_year and end\_year; equivalent to ESMValTool's syntax on multiple experiments; this option needs an ensemble to be declared explicitly; it will return no entry if there are gaps in data;
- start\_year and end\_year are required and are used to filter out the datasets that don't have data in the interval; as noted above, the tool will not return datasets with partial coverage from start\_year to end\_year; if you want all possible years hence no filtering on years just use "\*" for start and end years;
- config-user: rootpath: CMIPX may be a list, rootpath lists are supported;
- all major DRS paths (including default, BADC, ETHZ etc) are supported;
- speedup is achieved through CMIP mip tables lookup, so mip is required in recipe;

# 51.2 Caveats

- the tool doesn't yet work with derived variables; it will not return any available datasets;
- operation restricted to CMIP data only, OBS lookup is not available yet.

# CHAPTER

**FIFTYTWO** 

# **EXTRACTING A LIST OF INPUT FILES FROM THE PROVENANCE**

There is a small tool available to extract just the list of input files used to generate a figure from the \*\_provenance.xml files (see *Recording provenance* for more information).

To use it, install ESMValTool from source and run

python esmvaltool/utils/prov2files.py /path/to/result\_provenance.xml

The tool is based on the prov library, a useful library for working with provenance files. With minor adaptations, this script could also print out global attributes of the input NetCDF files, e.g. the tracking\_id.

# Part X

# **ESMValTool Code API Documentation**

ESMValTool is mostly used as a command line tool. However, it is also possible to use (parts of) ESMValTool as a library. This section documents the public API of ESMValTool.

# CHAPTER

# FIFTYTHREE

# SHARED DIAGNOSTIC CODE

# 53.1 Shared diagnostic script code

Code that is shared between multiple diagnostic scripts.

**Classes:** 

Datasets(cfg)	Class to easily access a recipe's datasets in a diagnostic script.
ProvenanceLogger(cfg)	Open the provenance logger.
Variable(short_name, standard_name,)	Variable class containing all relevant information.
Variables([cfg])	Class to easily access a recipe's variables in a diagnostic.

# **Functions:**

<pre>apply_supermeans(ctrl, exper, obs_list)</pre>	Apply supermeans on data components ie MEAN on time.
<pre>extract_variables(cfg[, as_iris])</pre>	Extract basic variable information from configuration dictionary.
<pre>get_cfg([filename])</pre>	Read diagnostic script configuration from settings.yml.
<pre>get_control_exper_obs(short_name,[,])</pre>	Get control, exper and obs datasets.
<pre>get_diagnostic_filename(basename, cfg[,])</pre>	Get a valid path for saving a diagnostic data file.
<pre>get_plot_filename(basename, cfg)</pre>	Get a valid path for saving a diagnostic plot.
<pre>group_metadata(metadata, attribute[, sort])</pre>	Group metadata describing preprocessed data by at- tribute.
<pre>run_diagnostic()</pre>	Run a Python diagnostic.
<pre>save_data(basename, provenance, cfg, cube,)</pre>	Save the data used to create a plot to file.
<pre>save_figure(basename, provenance, cfg[,])</pre>	Save a figure to file.
<pre>select_metadata(metadata, **attributes)</pre>	Select specific metadata describing preprocessed data.
<pre>sorted_group_metadata(metadata_groups, sort)</pre>	Sort grouped metadata.
<pre>sorted_metadata(metadata, sort)</pre>	Sort a list of metadata describing preprocessed data.
<pre>variables_available(cfg, short_names)</pre>	Check if data from certain variables is available.

# class esmvaltool.diag\_scripts.shared.Datasets(cfg)

# Bases: object

Class to easily access a recipe's datasets in a diagnostic script.

Note: This class has been deprecated in version 2.2 and will be removed two minor releases later in version 2.4.

# **Examples**

Get all variables of a recipe configuration *cfg*:

datasets = Datasets(cfg)

Access data of a dataset with path *dataset\_path*:

datasets.get\_data(path=dataset\_path)

Access dataset information of the dataset:

datasets.get\_dataset\_info(path=dataset\_path)

Access the data of all datasets with *exp=piControl*:

datasets.get\_data\_list(exp=piControl)

# Methods:

add_dataset(path[, data])	Add dataset to class.
<pre>add_to_data(data[, path])</pre>	Add element to a dataset's data.
<pre>get_data([path])</pre>	Access a dataset's data.
<pre>get_data_list(**dataset_info)</pre>	Access the datasets' data in a list.
<pre>get_dataset_info([path])</pre>	Access a dataset's information.
<pre>get_dataset_info_list(**dataset_info)</pre>	Access dataset's information in a list.
<pre>get_info(key[, path])</pre>	Access a 'dataset_info`'s key.
<pre>get_info_list(key, **dataset_info)</pre>	Access dataset_info's key values.
<pre>get_path(**dataset_info)</pre>	Access a dataset's path.
<pre>get_path_list(**dataset_info)</pre>	Access dataset's paths in a list.
<pre>set_data(data[, path])</pre>	Set element as a dataset's data.

add\_dataset(path, data=None, \*\*dataset\_info)

Add dataset to class.

# Parameters

- **path** (*str*) (Unique) path to the dataset.
- **data** (*optional*) Arbitrary object to be saved as data for the dataset.
- **\*\*dataset\_info** (*optional*) Keyword arguments describing the dataset, e.g. dataset=CanESM2, exp=piControl or short\_name=tas.

add\_to\_data(data, path=None, \*\*dataset\_info)

Add element to a dataset's data.

#### Notes

Either *path* or a unique *dataset\_info* description have to be given. Fails when given information is ambiguous.

# **Parameters**

- data Element to be added to the dataset's data.
- **path** (*str*, *optional*) Path to the dataset
- **\*\*dataset\_info** (optional) Keyword arguments describing the dataset, e.g. dataset=CanESM2, exp=piControl or short\_name=tas.

#### Raises

**RuntimeError** – If data given by *dataset\_info* is ambiguous.

# get\_data(path=None, \*\*dataset\_info)

Access a dataset's data.

#### Notes

Either *path* or a unique *dataset\_info* description have to be given. Fails when given information is ambiguous.

#### **Parameters**

- **path** (*str*, *optional*) Path to the dataset
- **\*\*dataset\_info** (optional) Keyword arguments describing the dataset, e.g. dataset=CanESM2, exp=piControl or short\_name=tas.

# Returns

Data of the selected dataset.

#### **Return type**

data\_object

# Raises

RuntimeError – If data given by dataset\_info is ambiguous.

# get\_data\_list(\*\*dataset\_info)

Access the datasets' data in a list.

### **Notes**

The returned data is sorted alphabetically respective to the *paths*.

#### Parameters

```
**dataset_info (optional) – Keyword arguments describing the dataset, e.g. dataset=CanESM2, exp=piControl or short_name=tas.
```

# Returns

Data of the selected datasets.

#### **Return type**

list

#### get\_dataset\_info(path=None, \*\*dataset\_info)

Access a dataset's information.

#### Notes

Either *path* or a unique *dataset\_info* description have to be given. Fails when given information is ambiguous.

#### **Parameters**

- **path** (*str*, *optional*) Path to the dataset.
- **\*\*dataset\_info** (optional) Keyword arguments describing the dataset, e.g. dataset=CanESM2, exp=piControl or short\_name=tas.

# Returns

All dataset information.

Return type

dict

# Raises

**RuntimeError** – If data given by *dataset\_info* is ambiguous.

# get\_dataset\_info\_list(\*\*dataset\_info)

Access dataset's information in a list.

# Notes

The returned data is sorted alphabetically respective to the *paths*.

#### Parameters

**\*\*dataset\_info** (*optional*) – Keyword arguments describing the dataset, e.g. *dataset=CanESM2*, *exp=piControl* or *short\_name=tas*.

#### Returns

Information dictionaries of the selected datasets.

Return type

list

# get\_info(key, path=None, \*\*dataset\_info)

Access a 'dataset\_info`'s key.

# Notes

Either *path* or a unique *dataset\_info* description have to be given. Fails when given information is ambiguous. If the *dataset\_info* does not contain the *key*, returns None.

#### Parameters

- key (str) Desired dictionary key.
- **path** (*str*) Path to the dataset.
- **\*\*dataset\_info** (*optional*) Keyword arguments describing the dataset, e.g. dataset=CanESM2, exp=piControl or short\_name=tas.

#### Returns

key information of the given dataset.

#### **Return type**

str

#### Raises

**RuntimeError** – If data given by *dataset\_info* is ambiguous.

# get\_info\_list(key, \*\*dataset\_info)

Access dataset\_info's key values.

# Notes

The returned data is sorted alphabetically respective to the *paths*.

#### **Parameters**

- **key** (*str*) Desired dictionary key.
- **\*\*dataset\_info** (optional) Keyword arguments describing the dataset, e.g. dataset=CanESM2, exp=piControl or short\_name=tas.

# Returns

key information of the selected datasets.

# Return type

list

# get\_path(\*\*dataset\_info)

Access a dataset's path.

#### Notes

A unique *dataset\_info* description has to be given. Fails when given information is ambiguous.

# Parameters

**\*\*dataset\_info** (*optional*) – Keyword arguments describing the dataset, e.g. *dataset=CanESM2*, *exp=piControl* or *short\_name=tas*.

#### Returns

Path of the selected dataset.

# **Return type**

str

#### Raises

**RuntimeError** – If data given by *dataset\_info* is ambiguous.

# get\_path\_list(\*\*dataset\_info)

Access dataset's paths in a list.

# Notes

The returned data is sorted alphabetically respective to the paths.

### **Parameters**

**\*\*dataset\_info** (*optional*) – Keyword arguments describing the dataset, e.g. *dataset=CanESM2*, *exp=piControl* or *short\_name=tas*.

#### Returns

Paths of the selected datasets.

Return type list

set\_data(data, path=None, \*\*dataset\_info)

Set element as a dataset's data.

#### Notes

Either *path* or a unique *dataset\_info* description have to be given. Fails when if given information is ambiguous.

#### **Parameters**

- **data** Element to be set as the dataset's data.
- **path** (*str*, *optional*) Path to the dataset.
- **\*\*dataset\_info** (*optional*) Keyword arguments describing the dataset, e.g. dataset=CanESM2, exp=piControl or short\_name=tas.

#### Raises

**RuntimeError** – If data given by *dataset\_info* is ambiguous.

class esmvaltool.diag\_scripts.shared.ProvenanceLogger(cfg)

# Bases: object

Open the provenance logger.

### Parameters

**cfg** (*dict*) – Dictionary with diagnostic configuration.

#### Example

Use as a context manager:

```
record = {
    'caption': "This is a nice plot.",
    'statistics': ['mean'],
    'domain': ['global'],
    'plot_type': ['zonal'],
    'authors': [
        'first_author',
        'second_author',
    ],
    'references':
        'author20journal',
    ],
    'ancestors': [
        '/path/to/input_file_1.nc',
        '/path/to/input_file_2.nc',
    ],
}
output_file = '/path/to/result.nc'
with ProvenanceLogger(cfg) as provenance_logger:
    provenance_logger.log(output_file, record)
```

Methods:

#### *log*(filename, record) Record provenance.

#### log(filename, record)

Record provenance.

#### **Parameters**

- filename (str) Name of the file containing the diagnostic data.
- record (dict) Dictionary with the provenance information to be logged.

# Typical keys are:

- ancestors
- authors
- caption
- domain
- plot\_type
- references
- statistics

Note: See the provenance documentation for more information.

class esmvaltool.diag\_scripts.shared.Variable(short\_name, standard\_name, long\_name, units)

# Bases: Variable

Variable class containing all relevant information.

Note: This class has been deprecated in version 2.2 and will be removed two minor releases later in version 2.4.

# Methods:

<pre>count(value, /)</pre>	Return number of occurrences of value.
<pre>index(value[, start, stop])</pre>	Return first index of value.

# Attributes:

long_name	Alias for field number 2
short_name	Alias for field number 0
standard_name	Alias for field number 1
units	Alias for field number 3

count(value,/)

Return number of occurrences of value.

**index**(*value*, *start*=0, *stop*=9223372036854775807,/)

Return first index of value.

Raises ValueError if the value is not present.

# long\_name

Alias for field number 2

# short\_name

Alias for field number 0

# standard\_name

Alias for field number 1

# units

Alias for field number 3

```
class esmvaltool.diag_scripts.shared.Variables(cfg=None, **names)
```

Bases: object

Class to easily access a recipe's variables in a diagnostic.

Note: This class has been deprecated in version 2.2 and will be removed two minor releases later in version 2.4.

# **Examples**

Get all variables of a recipe configuration cfg:

```
variables = Variables(cfg)
```

Access information of a variable *tas*:

```
variables.short_name('tas')
variables.standard_name('tas')
variables.long_name('tas')
variables.units('tas')
```

Access iris-suitable dictionary of a variable *tas*:

variables.iris\_dict('tas')

Check if variables *tas* and *pr* are available:

variables.vars\_available('tas', 'pr')

# Methods:

add_vars(**names)	Add custom variables to the class.
<pre>iris_dict(var)</pre>	Access iris dictionary of the variable.
long_name(var)	Access long name.
<pre>modify_var(var, **names)</pre>	Modify an already existing variable of the class.
<pre>short_name(var)</pre>	Access short name.
<pre>short_names()</pre>	Get list of all <i>short_names</i> .
<pre>standard_name(var)</pre>	Access standard name.
<pre>standard_names()</pre>	Get list of all <i>standard_names</i> .
units(var)	Access units.
<pre>var_name(var)</pre>	Access var name.
<pre>vars_available(*args)</pre>	Check if given variables are available.

#### add\_vars(\*\*names)

Add custom variables to the class.

# Parameters

**\*\*names** (dict or Variable, optional) – Keyword arguments of the form short\_name=Variable\_object where Variable\_object can be given as dict or Variable.

# iris\_dict(var)

Access **iris** dictionary of the variable.

#### Parameters

**var** (*str*) – (Short) name of the variable.

#### Returns

Dictionary containing all attributes of the variable which can be used directly in iris (*short\_name* replaced by *var\_name*).

# **Return type**

dict

# long\_name(var)

Access long name.

# Parameters

**var** (*str*) – (Short) name of the variable.

#### Returns

Long name of the variable.

# **Return type**

str

# modify\_var(var, \*\*names)

Modify an already existing variable of the class.

# **Parameters**

- **var** (*str*) (Short) name of the existing variable.
- **\*\*names** Keyword arguments of the form *short\_name=tas*.

#### Raises

- ValueError If var is not an existing variable.
- **TypeError** If a non-valid keyword argument is given.

# short\_name(var)

Access short name.

#### **Parameters**

**var** (*str*) – (Short) name of the variable.

#### Returns

Short name of the variable.

# **Return type**

str

### short\_names()

Get list of all *short\_names*.

#### Returns

List of all *short\_names*.

# Return type

list

# standard\_name(var)

Access standard name.

# Parameters

**var** (*str*) – (Short) name of the variable.

#### Returns

Standard name of the variable.

### **Return type**

str

# standard\_names()

Get list of all *standard\_names*.

# Returns

List of all *standard\_names*.

# Return type

list

# units(var)

Access units.

**Parameters var** (*str*) – (Short) name of the variable.

# Returns

Units of the variable.

# **Return type**

str

# var\_name(var)

Access var name.

# Parameters

**var** (*str*) – (Short) name of the variable.

### Returns

Var name (=short name) of the variable.

# **Return type**

str

# vars\_available(\*args)

Check if given variables are available.

# Parameters

\*args – Short names of the variables to be tested.

# Returns

True if variables are available, False if not.

# **Return type**

bool

esmvaltool.diag\_scripts.shared.apply\_supermeans(ctrl, exper, obs\_list)

Apply supermeans on data components ie MEAN on time.

This function is an extension of climate\_statistics() meant to ease the time-meaning procedure when dealing with CONTROL, EXPERIMENT and OBS (if any) datasets. ctrl: dictionary of CONTROL dataset exper: dictionary of EXPERIMENT dataset obs\_lis: list of dicts for OBS datasets (0, 1 or many)

Returns: control and experiment cubes and list of obs cubes

esmvaltool.diag\_scripts.shared.extract\_variables(cfg, as\_iris=False)

Extract basic variable information from configuration dictionary.

Returns *short\_name*, *standard\_name*, *long\_name* and *units* keys for each variable.

# Parameters

- cfg (dict) Diagnostic script configuration.
- **as\_iris** (*bool*, *optional*) Replace *short\_name* by *var\_name*, this can be used directly in iris classes.

#### Returns

Variable information in dict`s (values) for each `short\_name (key).

# **Return type**

dict

esmvaltool.diag\_scripts.shared.get\_cfg(filename=None)

Read diagnostic script configuration from settings.yml.

```
esmvaltool.diag_scripts.shared.get_control_exper_obs(short_name, input_data, cfg, cmip_type=None)
```

Get control, exper and obs datasets.

This function is used when running recipes that need a clear distinction between a control dataset, an experiment dataset and have optional obs (OBS, obs4MIPs etc) datasets; such recipes include recipe\_validation, and all the autoassess ones; short\_name: variable short name input\_data: dict containing the input data info cfg: config file as used in this module cmip\_type: optional, CMIP project type (CMIP5 or CMIP6)

esmvaltool.diag\_scripts.shared.get\_diagnostic\_filename(basename, cfg, extension='nc')

Get a valid path for saving a diagnostic data file.

# **Parameters**

- **basename** (*str*) The basename of the file.
- **cfg** (*dict*) Dictionary with diagnostic configuration.
- **extension** (*str*) File name extension.

### Returns

A valid path for saving a diagnostic data file.

#### **Return type**

str

esmvaltool.diag\_scripts.shared.get\_plot\_filename(basename, cfg)

Get a valid path for saving a diagnostic plot.

# Parameters

- **basename** (*str*) The basename of the file.
- **cfg** (*dict*) Dictionary with diagnostic configuration.

#### Returns

A valid path for saving a diagnostic plot.

# **Return type**

str

esmvaltool.diag\_scripts.shared.group\_metadata(metadata, attribute, sort=None)

Group metadata describing preprocessed data by attribute.

#### **Parameters**

- metadata (list of dict) A list of metadata describing preprocessed data.
- **attribute** (*str*) The attribute name that the metadata should be grouped by.
- **sort** See *sorted\_group\_metadata*.

#### Returns

A dictionary containing the requested groups.

#### **Return type**

dict of list of dict

```
esmvaltool.diag_scripts.shared.run_diagnostic()
```

Run a Python diagnostic.

This context manager is the main entry point for most Python diagnostics.

# Example

See esmvaltool/diag\_scripts/examples/diagnostic.py for an extensive example of how to start your diagnostic.

Basic usage is as follows, add these lines at the bottom of your script:

```
def main(cfg):
    # Your diagnostic code goes here.
    print(cfg)

if ___name__ == '___main__':
    with run_diagnostic() as cfg:
        main(cfg)
```

The *cfg* dict passed to *main* contains the script configuration that can be used with the other functions in this module.

esmvaltool.diag\_scripts.shared.save\_data(basename, provenance, cfg, cube, \*\*kwargs)

Save the data used to create a plot to file.

#### Parameters

- **basename** (*str*) The basename of the file.
- provenance (dict) The provenance record for the data.
- **cfg** (*dict*) Dictionary with diagnostic configuration.
- cube (iris.cube.Cube) Data cube to save.
- **\*\*kwargs** Extra keyword arguments to pass to iris.save.

See also:

#### ProvenanceLogger

For an example provenance record that can be used with this function.

Save a figure to file.

#### Parameters

- **basename** (*str*) The basename of the file.
- **provenance** (*dict*) The provenance record for the figure.
- **cfg** (*dict*) Dictionary with diagnostic configuration.
- **figure** (*matplotlib.figure.Figure*) Figure to save.
- **close** (*bool*) Close the figure after saving.
- **\*\*kwargs** Keyword arguments to pass to matplotlib.figure.Figure.savefig.

# See also:

#### ProvenanceLogger

For an example provenance record that can be used with this function.

#### esmvaltool.diag\_scripts.shared.select\_metadata(metadata, \*\*attributes)

Select specific metadata describing preprocessed data.

# **Parameters**

- metadata (list of dict) A list of metadata describing preprocessed data.
- **\*\*attributes** Keyword arguments specifying the required variable attributes and their values. Use the value '\*' to select any variable that has the attribute.

# Returns

A list of matching metadata.

#### **Return type**

list of dict

#### esmvaltool.diag\_scripts.shared.sorted\_group\_metadata(metadata\_groups, sort)

Sort grouped metadata.

Sorting is done on strings and is not case sensitive.

# Parameters

- **metadata\_groups** (dict of list of dict) Dictionary containing the groups of metadata.
- **sort** (bool or str or list of str) One or more attributes to sort by or True to just sort the groups but not the lists.

# Returns

A dictionary containing the requested groups.

#### **Return type**

dict of list of dict

esmvaltool.diag\_scripts.shared.sorted\_metadata(metadata, sort)

Sort a list of metadata describing preprocessed data.

Sorting is done on strings and is not case sensitive.

#### Parameters

- metadata (list of dict) A list of metadata describing preprocessed data.
- **sort** (str or list of str) One or more attributes to sort by.

#### Returns

The sorted list of variable metadata.

#### Return type

list of dict

esmvaltool.diag\_scripts.shared.variables\_available(cfg, short\_names)

Check if data from certain variables is available.

#### **Parameters**

- **cfg** (*dict*) Diagnostic script configuration.
- **short\_names** (*list of str*) Variable *short\_names* which should be checked.

#### Returns

True if all variables available, False if not.

# Return type bool

# 53.1.1 Iris helper functions

Convenience functions for iris objects.

# **Functions:**

<pre>check_coordinate(cubes, coord_name)</pre>	Compare coordinate of cubes and raise error if not iden- tical.
<pre>convert_to_iris(dict_)</pre>	Change all appearances of short_name to var_name.
<pre>get_mean_cube(datasets)</pre>	Get mean cube of a list of datasets.
<pre>intersect_dataset_coordinates(cubes)</pre>	Compare dataset coordinates of cubes and match them if necessary.
<pre>iris_project_constraint(projects, input_data)</pre>	Create iris.Constraint to select specific projects from data.
<pre>prepare_cube_for_merging(cube, cube_label)</pre>	Prepare single iris.cube.Cube in order to merge it later.
<pre>unify_1d_cubes(cubes, coord_name)</pre>	Unify 1D cubes by transforming them to identical coordinates.
<pre>unify_time_coord(cube[, target_units])</pre>	Unify time coordinate of cube in-place.

esmvaltool.diag\_scripts.shared.iris\_helpers.check\_coordinate(cubes, coord\_name)

Compare coordinate of cubes and raise error if not identical.

#### **Parameters**

• cubes (iris.cube.CubeList) – Cubes to be compared.

• coord\_name (str) – Name of the coordinate.

# Returns

Points of the coordinate.

# Return type

numpy.array

# Raises

- iris.exceptions.CoordinateNotFoundError Coordinate coord\_name is not a coordinate of one of the cubes.
- ValueError Given coordinate differs for the input cubes.

#### esmvaltool.diag\_scripts.shared.iris\_helpers.convert\_to\_iris(dict\_)

Change all appearances of short\_name to var\_name.

#### Parameters

**dict** (*dict*) – Dictionary to convert.

#### Returns

Converted dictionary.

### **Return type**

dict

#### Raises

KeyError – dict contains keys```short\_name'`` and 'var\_name'.

#### esmvaltool.diag\_scripts.shared.iris\_helpers.get\_mean\_cube(datasets)

Get mean cube of a list of datasets.

# **Parameters**

datasets (list of dict) – List of datasets (given as metadata dict).

#### Returns

Mean cube.

#### **Return type**

iris.cube.Cube

#### esmvaltool.diag\_scripts.shared.iris\_helpers.intersect\_dataset\_coordinates(cubes)

Compare dataset coordinates of cubes and match them if necessary.

Use intersection of coordinate 'dataset' of all given cubes and remove elements which are not given in all cubes.

#### Parameters

cubes (iris.cube.CubeList) - Cubes to be compared.

#### Returns

Transformed cubes.

# **Return type**

iris.cube.CubeList

# Raises

- iris.exceptions.CoordinateNotFoundError Coordinate dataset is not a coordinate of one of the cubes.
- **ValueError** At least one of the cubes contains a dataset coordinate with duplicate elements or the cubes do not share common elements.

Create iris. Constraint to select specific projects from data.

#### Parameters

- projects (list of str) Projects to be selected.
- **input\_data** (*list of dict*) List of dataset metadata used to extract all relevant datasets belonging to given projects.
- **negate** (*bool*, *optional* (*default: False*)) Negate constraint (False: select all elements that fit projects, *True* `: select all elements that do **not** fit projects).

### Returns

constraint for coordinate dataset.

#### **Return type**

iris.Constraint

esmvaltool.diag\_scripts.shared.iris\_helpers.prepare\_cube\_for\_merging(cube, cube\_label)
Prepare single iris.cube.Cube in order to merge it later.

### Parameters

- **cube** (*iris.cube.Cube*) Cube to be pre-processed.
- **cube\_label** (*str*) Label for the new scalar coordinate cube\_label.

esmvaltool.diag\_scripts.shared.iris\_helpers.unify\_1d\_cubes(cubes, coord\_name)

Unify 1D cubes by transforming them to identical coordinates.

Use union of all coordinates as reference and transform other cubes to it by adding missing values.

#### **Parameters**

- cubes (iris.cube.CubeList) Cubes to be processed.
- **coord\_name** (*str*) Name of the coordinate.

#### Returns

Transformed cubes.

#### **Return type**

iris.cube.CubeList

#### Raises

**ValueError** – Cubes are not 1D, coordinate name differs or not all cube coordinates are subsets of longest coordinate.

Unify time coordinate of cube in-place.

#### Parameters

- cube (*iris.cube.Cube*) Cube whose time coordinate is transformed in-place.
- target\_units (*str or cf\_units.Unit, optional*) Target time units.

#### Raises

iris.exceptions.CoordinateNotFoundError - Cube does not contain coordinate time.

# 53.1.2 Plotting

Module that provides common plot functions.

# **Functions:**

<pre>get_dataset_style(dataset[, style_file])</pre>	Retrieve the style information for the given dataset.
<pre>get_path_to_mpl_style([style_file])</pre>	Get path to matplotlib style file.
<pre>global_contourf(cube[, cbar_center,])</pre>	Plot global filled contour plot.
<pre>global_pcolormesh(cube[, cbar_center,])</pre>	Plot global color mesh.
<pre>multi_dataset_scatterplot(x_data, y_data,)</pre>	Plot a multi dataset scatterplot.
<pre>quickplot(cube, plot_type[, filename])</pre>	Plot a cube using one of the iris.quickplot functions.
<pre>scatterplot(x_data, y_data, filepath, **kwargs)</pre>	Plot a scatterplot.

esmvaltool.diag\_scripts.shared.plot.get\_dataset\_style(dataset, style\_file=None)

Retrieve the style information for the given dataset.

```
esmvaltool.diag_scripts.shared.plot.get_path_to_mpl_style(style_file=None)
Get path to matplotlib style file.
```

Plot global filled contour plot.

Note: This is only possible if the cube is 2D with dimensional coordinates *latitude* and *longitude*.

### **Parameters**

- cube (iris.cube.Cube) Cube to plot.
- **cbar\_center** (*float*, *optional*) Central value for the colormap, useful for diverging colormaps. Can only be used if **cbar\_range** is given.
- cbar\_label (str, optional) Label for the colorbar.
- **cbar\_range** (*list of float*, *optional*) Range of the colorbar (first and second list element) and number of distinct colors (third element). See numpy.linspace.
- cbar\_ticks (list, optional) Ticks for the colorbar.
- **\*\*kwargs** Keyword argument for iris.plot.contourf().

### Returns

Plot object.

# Return type

matplotlib.contour.QuadContourSet

# Raises

- **iris.exceptions.CoordinateNotFoundError** Input iris.cube.Cube does not contain the necessary dimensional coordinates 'latitude' and 'longitude'.
- ValueError Input iris.cube.Cube is not 2D.

Plot global color mesh.

Note: This is only possible if the cube is 2D with dimensional coordinates latitude and longitude.

#### Parameters

- cube (*iris.cube.Cube*) Cube to plot.
- **cbar\_center** (*float*, *optional*) Central value for the colormap, useful for diverging colormaps. Can only be used if vmin and vmax are given.
- **cbar\_label** (*str*, *optional*) Label for the colorbar.
- **cbar\_ticks** (*list*, *optional*) Ticks for the colorbar.
- **\*\*kwargs** Keyword argument for iris.plot.pcolormesh().

### Returns

Plot object.

#### **Return type**

matplotlib.contour.QuadContourSet

#### Raises

- iris.exceptions.CoordinateNotFoundError Input iris.cube.Cube does not contain the necessary dimensional coordinates 'latitude' and 'longitude'.
- ValueError Input iris.cube.Cube is not 2D.

Plot a multi dataset scatterplot.

# Notes

Allowed keyword arguments:

- *mpl\_style\_file* (str): Path to the matplotlib style file.
- *dataset\_style\_file* (str): Path to the dataset style file.
- plot\_kwargs (array-like): Keyword arguments for the plot (e.g. label, makersize, etc.).
- *save\_kwargs* (dict): Keyword arguments for saving the plot.
- axes\_functions (dict): Arbitrary functions for axes, i.e. axes.set\_title('title').

# **Parameters**

- **x\_data** (*array-like*) x data of each dataset.
- **y\_data** (*array-like*) y data of each dataset.
- datasets (array-like) Names of the datasets.
- **filepath** (*str*) Path to which plot is written.
- **\*\*kwargs** Keyword arguments.

# Raises

- **TypeError** A non-valid keyword argument is given or *x\_data*, *y\_data*, *datasets* or (if given) *plot\_kwargs* is not array-like.
- **ValueError** *x\_data*, *y\_data*, *datasets* or *plot\_kwargs* do not have the same size.
- esmvaltool.diag\_scripts.shared.plot.quickplot(cube, plot\_type, filename=None, \*\*kwargs)
  Plot a cube using one of the iris.quickplot functions.

esmvaltool.diag\_scripts.shared.plot.scatterplot(x\_data, y\_data, filepath, \*\*kwargs)
Plot a scatterplot.

# Notes

Allowed keyword arguments:

- *mpl\_style\_file* (str): Path to the matplotlib style file.
- plot\_kwargs (array-like): Keyword arguments for the plot (e.g. label, makersize, etc.).
- *save\_kwargs* (dict): Keyword arguments for saving the plot.
- axes\_functions (dict): Arbitrary functions for axes, i.e. axes.set\_title('title').

# Parameters

- **x\_data** (*array-like*) x data of each dataset.
- **y\_data** (*array-like*) y data of each dataset.
- **filepath** (*str*) Path to which plot is written.
- **\*\*kwargs** Keyword arguments.

# Raises

- **TypeError** A non-valid keyword argument is given or *x\_data*, *y\_data* or (if given) *plot\_kwargs* is not array-like.
- **ValueError** *x\_data*, *y\_data* or *plot\_kwargs* do not have the same size.

# CHAPTER

# FIFTYFOUR

# **DIAGNOSTIC SCRIPTS**

# 54.1 Emergent constraints diagnostics

This module provides various tools to evaluate emergent constraints for arbitrary input variables.

# 54.1.1 Examples

- Emergent constraints for equilibrium climate sensitivity
- Emergent constraint on equilibrium climate sensitivity from global temperature variability
- Emergent constraints on equilibrium climate sensitivity in CMIP5: do they hold for CMIP6?

# 54.1.2 Diagnostic scripts

# Emergent constraint on ECS from global temperature variability

Diagnostic script to reproduce emergent constraint of Cox et al. (2018).

# Description

Plot equilibrium climate sensitivity ECS vs. temperature variability metric to establish an emergent relationship for ECS.

# Author

Manuel Schlund (DLR, Germany)

# Project

CRESCENDO

# **Configuration options in recipe**

# confidence\_level: float, optional (default: 0.66) Confidence level for ECS error estimation.

# Calculation of emergent constraints on ECS

Diagnostic script to calculate various emergent constraints for ECS.

# Description

Calculate the X axis of various emergent constraints for the equilibrium climate sensitivity (ECS).

# Author

Manuel Schlund (DLR, Germany)

# Project

CRESCENDO

# **Configuration options in recipe**

# diag: str

Emergent constraint to calculate (must be one of 'brient\_shal', 'su', 'volodin', 'zhai').

### metric: str, optional (default: 'regression\_slope')

Metric to measure model error. Only relevant for Su et al. (2014) constraint. Must be one of 'regression\_slope', 'correlation\_coefficient'.

# n\_jobs: int, optional (default: 1)

Maximum number of jobs spawned by this class.

# output\_attributes: dict, optional

Write additional attributes to netcdf files.

# pattern: str, optional

Pattern matched against ancestor file names.

# savefig\_kwargs: dict

Keyword arguments for matplotlib.pyplot.savefig().

# seaborn\_settings: dict

Options for seaborn.set\_theme() (affects all plots).

# Evaluate multiple emergent constraints simultaneously

Diagnostic script to evaluate multiple emergent constraints simultaneously.

# Description

Establish multiple emergent constraints for arbitrary input variables and an arbitrary target variable. All input datasets need to be one-dimensional and must include a coordinate 'dataset' or 'model' (thus, the data describes a single scalar value for each dataset). All input datasets must be marked with a var\_type (either feature, label, prediction\_input or prediction\_input\_error) and a tag, which describes the type of data. This diagnostic supports only a single tag for label and an arbitrary number of tag s for feature. For every tag, a 'reference\_dataset' can be specified, which will be automatically considered as prediction\_input. If reference\_dataset contains '|' (e.g. 'OBS1|OBS2'), multiple datasets are considered as prediction\_input (in this case 'OBS1' and 'OBS2').

# Author

Manuel Schlund (DLR, Germany)

# Project

CRESCENDO

# **Configuration options in recipe**

#### additional data: list of dict, optional

Additional datasets given as list of metadata.

#### all\_data\_label: str, optional (default: 'all')

Label used in plots when all input data is considered. Only relevant if group\_by is not used.

#### combine\_groups: bool, optional (default: False)

Add results to plots for data generated by combining the data of all individual groups.

#### confidence\_level: float, optional (default: 0.66)

Confidence level for estimation of target variable.

#### group\_by: str, optional

Group input data by an attribute (e.g. produces separate plots for the individual groups, etc.).

#### ignore\_patterns: list of str, optional

Patterns matched against ancestor files. Those files are ignored.

# merge\_identical\_pred\_input: bool, optional (default: True)

Use identical prediction\_input values as single value.

#### numbers\_as\_markers: bool, optional (default: False)

Use numbers as markers in scatterplots.

# patterns: list of str, optional

Patterns matched against ancestor files.

# plot\_regression\_line\_mean: bool, optional (default: False)

Plot means of regression lines in scatterplots.

#### read\_external\_file: str, optional

Read input datasets from external file given as absolute path or relative path. In the latter case, 'auxiliary\_data\_dir' from the user configuration file is used as base directory.

# savefig\_kwargs: dict

Keyword arguments for matplotlib.pyplot.savefig().

#### seaborn\_settings: dict

Options for seaborn.set\_theme() (affects all plots).

### Evaluate single emergent constraint

Diagnostic script to evaluate a single emergent constraint.

# Description

Establish a single emergent constraint for an arbitrary input variable and an arbitrary target variable. All input datasets need to be one-dimensional and must include a coordinate 'dataset' or 'model' (thus, the data describes a single scalar value for each dataset). All input datasets must be marked with a var\_type (either feature, label, prediction\_input or prediction\_input\_error) and a tag, which describes the type of data. This diagnostic supports only a single tag for label and feature. For every tag, a 'reference\_dataset' can be specified, which will be automatically considered as prediction\_input. If reference\_dataset contains '|' (e.g. 'OBS1|OBS2'), multiple datasets are considered as prediction\_input (in this case 'OBS1' and 'OBS2').

# Author

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### Project

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# **Configuration options in recipe**

#### additional\_data: list of dict, optional

Additional datasets given as list of metadata.

# all\_data\_label: str, optional (default: 'all')

Label used in plots when all input data is considered. Only relevant if group\_by is not used.

#### combine\_groups: bool, optional (default: False)

Add results to plots for data generated by combining the data of all individual groups.

#### confidence\_level: float, optional (default: 0.66)

Confidence level for estimation of target variable.

#### group\_by: str, optional

Group input data by an attribute (e.g. produces separate plots for the individual groups, etc.).

#### ignore\_patterns: list of str, optional

Patterns matched against ancestor files. Those files are ignored.

### merge\_identical\_pred\_input: bool, optional (default: True)

Use identical prediction\_input values as single value.

### numbers\_as\_markers: bool, optional (default: False)

Use numbers as markers in scatterplots.

# patterns: list of str, optional

Patterns matched against ancestor files.

# plot\_regression\_line\_mean: bool, optional (default: False)

Plot means of regression lines in scatterplots.

# read\_external\_file: str, optional

Read input datasets from external file given as absolute path or relative path. In the latter case, 'auxiliary\_data\_dir' from the user configuration file is used as base directory.

#### savefig\_kwargs: dict

Keyword arguments for matplotlib.pyplot.savefig().

# seaborn\_settings: dict

Options for seaborn.set\_theme() (affects all plots).

# 54.1.3 Auxiliary scripts

# Auxiliary functions for emergent constraints scripts

Convenience functions for emergent constraints diagnostics.

#### **Functions:**

<i>cdf</i> (data, pdf)	Calculate cumulative distribution function for a 1-
	dimensional PDF.
<pre>check_metadata(metadata[, allowed_var_types])</pre>	Check metadata.
<pre>combine_groups(groups)</pre>	Combine list of groups to a single str.
<pre>constraint_info_array(x_data, y_data,[,])</pre>	Get array with all relevant parameters of emergent con- straint.
<pre>create_simple_scatterplot(x_data, y_data,)</pre>	Create simple scatterplot of an emergent relationship (without saving).
<i>export_csv</i> (data_frame, attributes, basename, cfg)	Export CSV file.
<pre>get_caption(attributes, feature, label[, group])</pre>	Construct caption from plotting attributes for (feature, label) pair.
<pre>get_colors(cfg[, groups])</pre>	Get color palette.
<pre>get_constraint(x_data, y_data, obs_mean, obs_std)</pre>	Get constraint on target variable.
<pre>get_constraint_from_df(training_data,[,])</pre>	Get constraint on target variable from pandas. DataFrame.
<pre>get_groups(training_data[, add_combined_group])</pre>	Extract groups from training data.
<pre>get_input_data(cfg)</pre>	Extract input data.
<pre>get_input_files(cfg[, patterns, ignore_patterns])</pre>	Get input files.
<pre>get_provenance_record(attributes, tags, **kwargs)</pre>	Get provenance record.
<pre>get_xy_data_without_nans(data_frame,)</pre>	Get (X, Y) data for (feature, label) combination without nans.
<pre>pandas_object_to_cube(pandas_object[,])</pre>	Convert pandas object to iris.cube.Cube.
<pre>plot_individual_scatterplots(training_data,)</pre>	Plot individual scatterplots for the different groups.
<pre>plot_merged_scatterplots(training_data,)</pre>	Plot merged scatterplots (all groups in one plot).
<pre>plot_target_distributions(training_data,)</pre>	Plot distributions of target variable for every feature.
<pre>regression_line(x_data, y_data[, n_points])</pre>	Return x and y coordinates of the regression line (mean and error).
<pre>set_plot_appearance(axes, attributes, **kwargs)</pre>	Set appearance of a plot.
<pre>standard_prediction_error(x_data, y_data)</pre>	Return a function to calculate standard prediction error.
<pre>target_pdf(x_data, y_data, obs_mean, obs_std)</pre>	Calculate probability density function (PDF) for target variable.

esmvaltool.diag\_scripts.emergent\_constraints.cdf(data, pdf)

Calculate cumulative distribution function for a 1-dimensional PDF.

### **Parameters**

- data (numpy.ndarray) Data points (1D array).
- pdf (numpy.ndarray) Corresponding probability density function (PDF).

# Returns

Corresponding cumulative distribution function (CDF).

# **Return type**

numpy.ndarray

# Parameters

- **metadata** (*dict*) Metadata to check.
- **allowed\_var\_types** (*list of str, optional*) Allowed var\_types, defaults to ALLOWED\_VAR\_TYPES.

# Raises

- KeyError Metadata does not contain necessary keys 'var\_type' and 'tag'.
- ValueError Got invalid value for key 'var\_type'.

# esmvaltool.diag\_scripts.emergent\_constraints.combine\_groups(groups)

Combine list of groups to a single str.

# Parameters

**groups** (*list of str*) – List of group names.

#### Returns

Combined str.

#### **Return type**

str

necessary\_p\_value=None)

Get array with all relevant parameters of emergent constraint.

# Parameters

- **x\_data** (*numpy.ndarray*) X data of the emergent constraint.
- y\_data (numpy.ndarray) Y data of the emergent constraint.
- **obs\_mean** (*float*) Mean of observational data.
- **obs\_std** (*float*) Standard deviation of observational data.
- **n\_points** (*int*, *optional* (*default:* 1000)) Number of sampled points for PDF of target variable.
- **necessary\_p\_value** (*float*, *optional*) If given, replace constrained mean and standard deviation with unconstrained values when *p*-value of emergent relationship is greater than the given necessary *p*-value.

### Returns

# Array of shape (8,) with the elements:

- 0. Constrained mean of target variable.
- 1. Constrained standard deviation of target variable.
- 2. Unconstrained mean of target variable.
- 3. Unconstrained standard deviation of target variable.
- 4. Slope of emergent relationship.
- 5. Intercept of emergent relationship.
- 6. Correlation coefficient r of emergent relationship.
- 7. *p*-value of emergent relationship.

# **Return type**

numpy.ndarray

esmvaltool.diag\_scripts.emergent\_constraints.create\_simple\_scatterplot(x\_data, y\_data,

obs\_mean, obs\_std)

Create simple scatterplot of an emergent relationship (without saving).

#### **Parameters**

- **x\_data** (*numpy.ndarray*) X data of the emergent constraint.
- y\_data (numpy.ndarray) Y data of the emergent constraint.
- obs\_mean (float) Mean of observational data.
- obs\_std (float) Standard deviation of observational data.

#### Export CSV file.

# Parameters

- data\_frame (pandas.DataFrame) Data to export.
- **attributes** (*dict*) Plot attributes for the different features and the label data. Used to retrieve provenance information.
- **basename** (*str*) Basename for the name of the file.
- **cfg** (*dict*) Recipe configuration.
- **tags** (*iterable of str*, *optional*) Tags for which provenance information should be retrieved (using attributes). If not specified, use (last level of) columns of the given data\_frame.

#### Returns

Path to the new CSV file.

#### **Return type**

str

esmvaltool.diag\_scripts.emergent\_constraints.get\_caption(attributes, feature, label, group=None)
Construct caption from plotting attributes for (feature, label) pair.

#### **Parameters**

- attributes (dict) Plot attributes.
- **feature** (*str*) Feature.
- label (*str*) Label.
- group (str, optional) Group.

#### Returns

Caption.

#### **Return type**

str

# Raises

KeyError – attributes does not include necessary keys.

esmvaltool.diag\_scripts.emergent\_constraints.get\_colors(cfg, groups=None)

Get color palette.

#### **Parameters**

- **cfg** (*dict*) Recipe configuration.
- **groups** (*list*, *optional*) Use to check whether color for combining groups has to be added.

#### Returns

List of colors that can be used for matplotlib.

#### **Return type**

list

Get constraint on target variable.

#### Parameters

- **x\_data** (*numpy.ndarray*) X data of the emergent constraint.
- y\_data (*numpy.ndarray*) Y data of the emergent constraint.
- **obs\_mean** (*float*) Mean of observational data.
- **obs\_std** (*float*) Standard deviation of observational data.
- **confidence\_level** (*float*, *optional* (*default:* 0.66)) Confindence level to estimate the range of the target variable.

#### Returns

Lower confidence limit, best estimate and upper confidence limit of target variable.

#### **Return type**

tuple of float

esmvaltool.diag\_scripts.emergent\_constraints.get\_constraint\_from\_df(training\_data,

pred\_input\_data, confidence\_level=0.66)

Get constraint on target variable from pandas.DataFrame.

#### **Parameters**

- training\_data (pandas.DataFrame) Training data (features, label).
- pred\_input\_data (pandas.DataFrame) Prediction input data (mean and error).
- **confidence\_level** (*float*, *optional* (*default:* 0.66)) Confindence level to estimate the range of the target variable.

#### Returns

Lower confidence limit, best estimate and upper confidence limit of target variable.

#### **Return type**

tuple of float

esmvaltool.diag\_scripts.emergent\_constraints.get\_groups(training\_data,

add\_combined\_group=False)

Extract groups from training data.

# Parameters

- training\_data (pandas.DataFrame) Training data (features, label).
- add\_combined\_group (bool, optional (default: False)) Add combined group of all other groups at the beginning of the returned list.

#### Returns

Groups.

# Return type

list of str

esmvaltool.diag\_scripts.emergent\_constraints.get\_input\_data(cfg)

Extract input data.

Return training data, prediction input data and corresponding attributes.

Parameters

cfg (dict) – Recipe configuration.

#### Returns

A tuple containing the training data (pandas.DataFrame), the prediction input data (pandas. DataFrame) and the corresponding attributes (dict).

#### **Return type**

tuple

```
esmvaltool.diag_scripts.emergent_constraints.get_input_files(cfg, patterns=None,
```

ignore\_patterns=None)

Get input files.

#### **Parameters**

- **cfg** (*dict*) Recipe configuration.
- **patterns** (*list of str, optional*) Use only ancestor files that match these patterns as input files.
- **ignore\_patterns** (*list of str, optional*) Ignore input files that match these patterns.

#### Returns

Input files.

## **Return type**

list of str

esmvaltool.diag\_scripts.emergent\_constraints.get\_provenance\_record(attributes, tags, \*\*kwargs)
Get provenance record.

## Parameters

- **attributes** (*dict*) Plot attributes. All provenance keys need to start with 'provenance\_'.
- **tags** (*list of str*) Tags used to retrieve data from the attributes dict, i.e. features and/or label.
- **\*\*kwargs** (*Keyword arguments*) Additional key:value pairs directly passed to the provenance record dict. All values may include the format strings {feature} and {label}.

#### Returns

Provenance record.

#### **Return type**

dict

esmvaltool.diag\_scripts.emergent\_constraints.get\_xy\_data\_without\_nans(data\_frame, feature,

label)

Get (X, Y) data for (feature, label) combination without nans.

#### **Parameters**

• **data\_frame** (*pandas*.*DataFrame*) – Training data.

- feature (str) Name of the feature data.
- **label** (*str*) Name of the label data.

## Returns

Tuple containing a pandas.DataFrame for the X axis (feature) and a pandas.DataFrame for the Y axis (label) without missing values.

# **Return type**

tuple

```
esmvaltool.diag_scripts.emergent_constraints.pandas_object_to_cube(pandas_object,
```

index\_droplevel=None, columns\_droplevel=None, \*\*kwargs)

Convert pandas object to iris.cube.Cube.

#### Parameters

- pandas\_object (pandas.DataFrame or pandas.Series) Data to convert.
- **index\_droplevel** (*int or list of int, optional*) Drop levels of index if not None.
- **columns\_droplevel** (*int or list of int, optional*) Drop levels of columns if not None. Can only be used if pandas\_object is a pandas.DataFrame.
- **\*\*kwargs** (*Keyword arguments*) Keyword arguments used for the cube metadata, e.g. standard\_name, var\_name, etc.

#### Returns

Data cube.

#### **Return type**

iris.cube.Cube

#### Raises

**TypeError** – columns\_droplevel is used when pandas\_object is not a pandas. DataFrame.

basename, cfg)

Plot individual scatterplots for the different groups.

Plot scatterplots for all pairs of (feature, label) data (Separate plot for each group).

# Parameters

- training\_data (pandas.DataFrame) Training data (features, label).
- pred\_input\_data (pandas.DataFrame) Prediction input data (mean and error).
- **attributes** (*dict*) Plot attributes for the different features and the label data.
- **basename** (*str*) Basename for the name of the file.
- **cfg** (*dict*) Recipe configuration.

esmvaltool.diag\_scripts.emergent\_constraints.plot\_merged\_scatterplots(training\_data,

pred\_input\_data,
attributes, basename,
cfg)

Plot merged scatterplots (all groups in one plot).

Plot scatterplots for all pairs of (feature, label) data (all groups in one plot).

#### Parameters

- training\_data (pandas.DataFrame) Training data (features, label).
- pred\_input\_data (pandas.DataFrame) Prediction input data (mean and error).
- **attributes** (*dict*) Plot attributes for the different features and the label data.
- **basename** (*str*) Basename for the name of the file.
- **cfg** (*dict*) Recipe configuration.

esmvaltool.diag\_scripts.emergent\_constraints.plot\_target\_distributions(training\_data,

pred\_input\_data, attributes, basename, cfg)

Plot distributions of target variable for every feature.

## Parameters

- training\_data (pandas.DataFrame) Training data (features, label).
- pred\_input\_data (pandas.DataFrame) Prediction input data (mean and error).
- **attributes** (*dict*) Plot attributes for the different features and the label data.
- **basename** (*str*) Basename for the name of the file.
- **cfg** (*dict*) Recipe configuration.

esmvaltool.diag\_scripts.emergent\_constraints.regression\_line(x\_data, y\_data, n\_points=1000) Return x and y coordinates of the regression line (mean and error).

# **Parameters**

- **x\_data** (*numpy.ndarray*) X data used to fit the linear regression.
- y\_data (numpy.ndarray) Y data used to fit the linear regression.
- **n\_points** (*int*, *optional* (*default:* 1000)) Number of points for the regression lines.

#### Returns

```
numpy.ndarray s for the keys 'x', 'y', 'y_minus_err', 'y_plus_err', 'slope',
'intercept', 'pvalue' and 'rvalue'.
```

#### **Return type**

dict

esmvaltool.diag\_scripts.emergent\_constraints.set\_plot\_appearance(axes, attributes, \*\*kwargs)
Set appearance of a plot.

#### **Parameters**

- axes (matplotlib.axes.Axes) Matplotlib Axes object which contains the plot.
- attributes (*dict*) Plot attributes.
- **\*\*kwargs**(*Keyword arguments*) Keyword arguments of the form plot\_option=tag where plot\_option is something like plot\_title, plot\_xlabel, plot\_xlim, etc.

and tag a key for the plot attributes dict that describes which attributes should be considered for that plot\_option.

esmvaltool.diag\_scripts.emergent\_constraints.standard\_prediction\_error(x\_data, y\_data)

Return a function to calculate standard prediction error.

The standard prediction error of a linear regression is the error when predicting a data point which was not used to fit the regression line in the first place.

#### **Parameters**

- **x\_data** (*numpy.ndarray*) X data used to fit the linear regression.
- **y\_data** (*numpy.ndarray*) Y data used to fit the linear regression.

#### Returns

Function that takes a float as single argument (representing the X value of a new data point) and returns the standard prediction error for that.

#### **Return type**

callable

Calculate probability density function (PDF) for target variable.

#### Parameters

- **x\_data** (*numpy.ndarray*) X data of the emergent constraint.
- y\_data (numpy.ndarray) Y data of the emergent constraint.
- **obs\_mean** (*float*) Mean of observational data.
- **obs\_std** (*float*) Standard deviation of observational data.
- **n\_points** (*int*, *optional* (*default:* 1000)) Number of sampled points for PDF of target variable.
- **necessary\_p\_value** (*float*, *optional*) If given, return unconstrained PDF (using Gaussian distribution with unconstrained mean and standard deviation) when *p*-value of emergent relationship is greater than the given necessary *p*-value.

#### Returns

x and y values for the PDF.

#### **Return type**

tuple of numpy.ndarray

# 54.2 Machine Learning Regression (MLR) diagnostics

This module provides various tools to create and evaluate MLR models for arbitrary input variables.

# 54.2.1 Examples

• *Constraining uncertainty in projected gross primary production (GPP) with machine learning*: Use Gradient Boosted Regression Tree (GBRT) algorithm to constrain projected Gross Primary Production (GPP) in RCP 8.5 scenario using observations of process-based predictors.

# 54.2.2 Diagnostic scripts

# **Evaluate residuals**

Simple evaluation of residuals (coming from MLR model output).

## Description

This diagnostic evaluates residuals created by MLR models.

# **Author**

Manuel Schlund (DLR, Germany)

# Project

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# Configuration options in recipe

#### ignore: list of dict, optional

Ignore specific datasets by specifying multiple dict s of metadata.

# mse\_plot: dict, optional

Additional options for plotting the mean square errors (MSE). Specify additional keyword arguments for seaborn.boxplot() by plot\_kwargs and plot appearance options by pyplot\_kwargs (processed as functions of matplotlib.pyplot).

# pattern: str, optional

Pattern matched against ancestor file names.

#### rmse\_plot: dict, optional

Additional options for plotting the root mean square errors (RMSE). Specify additional keyword arguments for seaborn.boxplot() by plot\_kwargs and plot appearance options by pyplot\_kwargs (processed as functions of matplotlib.pyplot).

#### savefig\_kwargs: dict, optional

Keyword arguments for matplotlib.pyplot.savefig().

# seaborn\_settings: dict, optional

Options for seaborn.set\_theme() (affects all plots).

# weighted\_samples: dict

If specified, use weighted root mean square error. The given keyword arguments are directly passed to *esmvaltool.diag\_scripts.mlr.get\_all\_weights()* to calculate the sample weights. By default, area weights and time weights are used.

# **MLR** main diagnostic

Main Diagnostic script to create MLR models.

# **Description**

This diagnostic script creates Machine Learning Regression (MLR) models which use inter-model relations between process-based predictors (usually from the past/present climate) and a target variable (usually a projection of the future climate) to get a constrained prediction of the target variable. It provides an interface for using MLR models (subclasses of *esmvaltool.diag\_scripts.mlr.models.MLRModel*).

# Author

Manuel Schlund (DLR, Germany)

# Project

CRESCENDO

# **Configuration options in recipe**

# efecv\_kwargs: dict, optional

If specified, use these additional keyword arguments to perform a exhaustive feature elimination using cross-validation. May not be used together with grid\_search\_cv\_param\_grid or rfecv\_kwargs.

#### grid\_search\_cv\_kwargs: dict, optional

Keyword arguments for the grid search cross-validation, see https://scikit-learn.org/stable/modules/generated/sklearn.model\_selection.GridSearchCV.html.

#### grid\_search\_cv\_param\_grid: dict or list of dict, optional

If specified, perform exhaustive parameter search using cross-validation instead of simply calling *esmvaltool*. *diag\_scripts.mlr.models.MLRModel.fit()*. Contains parameters (keys) and ranges (values) for the exhaustive parameter search. Have to be given for each step of the pipeline separated by two underscores, i.e. s\_\_p is the parameter p for step s. May not be used together with efecv\_kwargs or rfecv\_kwargs.

#### group\_metadata: str, optional

Group input data by an attribute. For every group element (set of datasets), an individual MLR model is calculated. Only affects feature and label datasets. May be used together with the option pseudo\_reality.

#### ignore: list of dict, optional

Ignore specific datasets by specifying multiple dict s of metadata.

#### mlr\_model\_type: str

MLR model type. The given model has to be defined in *esmvaltool.diag\_scripts.mlr.models*.

#### only\_predict: bool, optional (default: False)

If True, only use *esmvaltool.diag\_scripts.mlr.models.MLRModel.predict()* and do not create any other output (CSV files, plots, etc.).

# pattern: str, optional

Pattern matched against ancestor file names.

# plot\_partial\_dependences: bool, optional (default: False)

Plot partial dependence of every feature in MLR model (computationally expensive).

# predict\_kwargs: dict, optional

Optional keyword arguments for the final regressor's predict() function.

# pseudo\_reality: list of str, optional

List of dataset attributes which are used to group input data for a pseudo- reality test (also known as *model-as-truth* or *perfect-model* setup). For every element of the group a single MLR model is fitted on all data **except** for that of the specified group element. This group element is then used as additional prediction\_input and prediction\_reference. This allows a direct assessment of the predictive power of the MLR model by comparing the MLR prediction output and the true labels (similar to splitting the input data in a training and test set, but not dividing the data randomly but using specific datasets, e.g. the different climate models). May be used together with the option group\_metadata.

# rfecv\_kwargs: dict, optional

If specified, use these additional keyword arguments to perform a recursive feature elimination using cross-validation, see <a href="https://scikit-learn.org/stable/modules/generated/sklearn.feature\_selection.RFECV.html">https://scikit-learn.org/stable/modules/generated/sklearn.feature\_selection.RFECV.html</a>. May not be used together with efecv\_kwargs or grid\_search\_cv\_param\_grid.

# save\_mlr\_model\_error: str or int, optional

Additionally saves estimated squared MLR model error. This error represents the uncertainty of the prediction caused by the MLR model itself and not by errors in the prediction input data (errors in that will be considered by including datasets with var\_type set to prediction\_input\_error and setting save\_propagated\_errors to True). If the option is set to 'test', the (constant) error is estimated as RMSEP using a (hold-out) test data set. Only possible if test data is available, i.e. the option test\_size is not set to False during class initialization. If the option is set to 'logo', the (constant) error is estimated as RMSEP using leave-one-group-out cross-validation using the group\_attributes. Only possible if group\_datasets\_by\_attributes is given. If the option is set to an integer n (!= 0), the (constant) error is estimated as RMSEP using n-fold cross-validation.

# save\_lime\_importance: bool, optional (default: False)

Additionally save local feature importance given by LIME (Local Interpretable Model-agnostic Explanations).

# save\_propagated\_errors: bool, optional (default: False)

Additionally save propagated errors from prediction\_input\_error datasets.

#### select\_metadata: dict, optional

Pre-select input data by specifying (key, value) pairs. Affects all datasets regardless of var\_type.

Additional optional parameters are optional parameters for *esmvaltool.diag\_scripts.mlr.models.MLRModel* given *here* or optional parameters of *esmvaltool.diag\_scripts.mlr.mmm* if mlr\_model\_type='mmm'.

# Multi-model means (MMM)

Use simple multi-model mean for predictions.

# Description

This diagnostic calculates the (unweighted) mean over all given datasets for a given target variable.

# Author

Manuel Schlund (DLR, Germany)

# Project

CRESCENDO

# **Configuration options in recipe**

#### convert\_units\_to: str, optional

Convert units of the input data. Can also be given as dataset option.

# dtype: str (default: 'float64')

Internal data type which is used for all calculations, see https://docs.scipy.org/doc/numpy/user/basics.types.html for a list of allowed values.

## ignore: list of dict, optional

Ignore specific datasets by specifying multiple dict s of metadata.

# mlr\_model\_name: str, optional (default: 'MMM')

Human-readable name of the MLR model instance (e.g used for labels).

#### mmm\_error\_type: str, optional

If given, additionally saves estimated squared MMM model error. If the option is set to 'loo', the (constant) error is estimated as RMSEP using leave-one-out cross-validation. No other options are supported at the moment.

# pattern: str, optional

Pattern matched against ancestor file names.

#### prediction\_name: str, optional

Default prediction\_name of output cubes if no 'prediction\_reference' dataset is given.

# weighted\_samples: dict

If specified, use weighted mean square error to estimate prediction error. The given keyword arguments are directly passed to *esmvaltool.diag\_scripts.mlr.get\_all\_weights()* to calculate the sample weights. By default, area weights and time weights are used.

## **Plotting functionalities**

Plotting scripts for MLR models input/output.

# Description

This diagnostic creates plots for MLR model input/output.

# Author

Manuel Schlund (DLR, Germany)

# Project

CRESCENDO

# Notes

All configuration options starting with plot\_ specify keyword arguments for a specific plot type. A certain plot type is only plotted if the corresponding option is given in the recipe (if no additional keyword arguments are desired, use {}).

# **Configuration options in recipe**

# additional\_plot\_kwargs\_xy\_plots: dict, optional

Optional keyword arguments (values) for single datasets used in X-Y plots. They keys may include a var\_type or values of the attribute given by group\_by\_attribute.

# alias: dict, optional

str to str mapping for nicer plot labels (e.g. {'feature': 'Historical CMIP5 data'}.

# apply\_common\_mask: bool, optional (default: False)

Apply common mask to all datasets prior to plotting. Requires identical shapes for all datasets.

# group\_attribute\_as\_default\_alias: bool, optional (default: True)

If True, use value of attribute given by group\_by\_attribute as default alias if possible. If False, use full group name (including var\_type) as default alias.

# group\_by\_attribute: str, optional (default: 'mlr\_model\_name')

By default, datasets are grouped using the var\_type attribute. This option can be used to specify a further attribute to group datasets. This diagnostic expects a single dataset per group.

# ignore: list of dict, optional

Ignore specific datasets by specifying multiple dict s of metadata.

# legend\_kwargs: dict, optional

Optional keyword arguments of matplotlib.pyplot.legend() (affects only plots with legends).

# map\_plot\_type: str, optional (default: 'pcolormesh')

Type of plot used for plotting maps. Must be one of 'pcolormesh' or 'contourf'.

#### pattern: str, optional

Pattern matched against ancestor file names.

#### plot\_map: dict, optional

Specify additional keyword arguments for plotting global maps showing datasets by plot\_kwargs and plot appearance options by pyplot\_kwargs (processed as functions of matplotlib.pyplot).

#### plot\_map\_abs\_biases: dict, optional

Specify additional keyword arguments for plotting global maps showing absolute biases by plot\_kwargs and plot appearance options by pyplot\_kwargs (processed as functions of matplotlib.pyplot).

# plot\_map\_ratios: dict, optional

Specify additional keyword arguments for plotting global maps showing ratios of datasets by plot\_kwargs and plot appearance options by pyplot\_kwargs (processed as functions of matplotlib.pyplot).

# plot\_map\_rel\_biases: dict, optional

Specify additional keyword arguments for plotting global maps showing relative biases of datasets by plot\_kwargs and plot appearance options by pyplot\_kwargs (processed as functions of matplotlib. pyplot).

# plot\_xy: dict, optional

Specify additional keyword arguments for simple X-Y plots by plot\_kwargs and plot appearance options by pyplot\_kwargs (processed as functions of matplotlib.pyplot). By default, plots data against dimensional coordinate (if available). Use x\_coord (str) to use another coordinate as X-axis. Use reg\_line: True to additionally plot a linear regression line.

# plot\_xy\_with\_errors: dict, optional

Specify additional keyword arguments for X-Y plots with error ranges plot\_kwargs and plot appearance options by pyplot\_kwargs (processed as functions of matplotlib.pyplot). By default, plots data against dimensional coordinate (if available). Use x\_coord (str) to use another coordinate as X-axis.

#### print\_corr: bool, optional (default: False)

Print and save Pearson correlation coefficient between all datasets at the end. Requires identical shapes for all datasets.

# savefig\_kwargs: dict, optional

Keyword arguments for matplotlib.pyplot.savefig().

# seaborn\_settings: dict, optional

Options for seaborn.set\_theme() (affects all plots).

# years\_in\_title: bool, optional (default: False)

Print years in default title of plots.

# **Postprocessing functionalities**

Simple postprocessing of MLR model output.

# Description

This diagnostic performs postprocessing operations for MLR model output (mean and error).

# Author

Manuel Schlund (DLR, Germany)

# Project

CRESCENDO

# Notes

Prior to postprocessing, this diagnostic groups input datasets according to tag and prediction\_name. For each group, accepts datasets with three different var\_type s:

- prediction\_output: Exactly one necessary, refers to the mean prediction and serves as reference dataset (regarding shape).
- prediction\_output\_error: Arbitrary number of error datasets. If not given, error calculation is skipped. May be squared errors (marked by the attribute squared) or not. In addition, a single covariance dataset can be specified (short\_name ending with \_cov).
- prediction\_input: Dataset used to estimate covariance structure of the mean prediction (i.e. matrix of Pearson correlation coefficients) for error estimation. At most one dataset allowed. Ignored when no prediction\_output\_error is given. This is only possible when (1) the shape of the prediction\_input dataset is identical to the shape of the prediction\_output\_error datasets, (2) the number of dimensions of the prediction\_input dataset is higher than the number of dimensions of the prediction\_output\_error datasets and they have identical trailing (rightmost) dimensions of prediction\_output\_error datasets and all dimensions of the prediction\_output\_error datasets are mapped to a corresponding dimension of the prediction\_input using the cov\_estimate\_dim\_map option (e.g. when prediction\_input has shape (10, 5, 100, 20) and prediction\_output\_error has shape (5, 20), you can use cov\_estimate\_dim\_map: [1, 3] to map the dimensions of prediction\_output\_error to dimension 1 and 3 of prediction\_input).

All data with other var\_type s is ignored (feature, label, etc.).

Real error calculation (using covariance dataset given as prediction\_output\_error) and estimation (using prediction\_input dataset to estimate covariance structure) is only possible if the mean prediction cube is collapsed completely during postprocessing, i.e. all coordinates are listed for either mean or sum.

# **Configuration options in recipe**

#### add\_var\_from\_cov: bool, optional (default: True)

Calculate variances from covariance matrix (diagonal elements) and add those to (squared) error datasets. Set to False if variance is already given separately in prediction output.

#### area\_weighted: bool, optional (default: True)

Calculate weighted averages/sums when collapsing over latitude and/or longitude coordinates using grid cell areas (calculated using grid cell bounds). Only possible for datasets on regular grids that contain latitude and longitude coordinates.

## convert\_units\_to: str, optional

Convert units of the input data.

#### cov\_estimate\_dim\_map: list of int, optional

Map dimensions of prediction\_output\_error datasets to corresponding dimensions of prediction\_input used for estimating covariance. Only relevant if both dataset types are given. See notes above for more information.

#### ignore: list of dict, optional

Ignore specific datasets by specifying multiple dict s of metadata.

# landsea\_fraction\_weighted: str, optional

When given, calculate weighted averages/sums when collapsing over latitude and/or longitude coordinates using land/sea fraction (calculated using Natural Earth masks). Only possible if the datasets contains latitude and longitude coordinates. Must be one of 'land', 'sea'.

# mean: list of str, optional

Perform mean over the given coordinates.

# pattern: str, optional

Pattern matched against ancestor file names.

**sum: list of str, optional** Perform sum over the given coordinates.

time\_weighted: bool, optional (default: True) Calculate weighted averages/sums for time (using time bounds).

# **Preprocessing functionalities**

Simple preprocessing of MLR model input.

# Description

This diagnostic performs preprocessing operations for datasets used as MLR model input in a desired way. It can also be used to process output of MLR models for plotting.

# Author

Manuel Schlund (DLR, Germany)

# Project

CRESCENDO

#### **Configuration options in recipe**

#### aggregate\_by: dict, optional

Aggregate over given coordinates (dict values; given as list of str) using a desired aggregator (dict key; given as str). Allowed aggregators are 'max', 'mean', 'median', 'min', 'sum', 'std', 'var', and 'trend'.

# apply\_common\_mask: bool, optional (default: False)

Apply common mask to all datasets. Requires identical shapes for all datasets.

#### area\_weighted: bool, optional (default: True)

Use weighted aggregation when collapsing over latitude and/or longitude using collapse. Weights are estimated using grid cell bounds. Only possible for datasets on regular grids that contain latitude and longitude coordinates.

#### argsort: dict, optional

Calculate numpy.ma.argsort() along given coordinate to get ranking. The coordinate can be specified by the coord key. If descending is set to True, use descending order instead of ascending.

# collapse: dict, optional

Collapse over given coordinates (dict values; given as list of str) using a desired aggregator (dict key; given as str). Allowed aggregators are 'max', 'mean', 'median', 'min', 'sum', 'std', 'var', and 'trend'.

#### convert\_units\_to: str, optional

Convert units of the input data. Can also be given as dataset option.

#### extract: dict, optional

Extract certain values (dict values, given as int, float or iterable of them) for certain coordinates (dict keys, given as str).

# extract\_ignore\_bounds: bool, optional (default: False)

If True, ignore coordinate bounds when using extract or extract\_range. If False, consider coordinate bounds when using extract or extract\_range. For time coordinates, bounds are always ignored.

#### extract\_range: dict, optional

Like extract, but instead of specific values extract ranges (dict values, given as iterable of exactly two int s or float s) for certain coordinates (dict keys, given as str).

# ignore: list of dict, optional

Ignore specific datasets by specifying multiple dict s of metadata.

#### landsea\_fraction\_weighted: str, optional

When given, use land/sea fraction for weighted aggregation when collapsing over latitude and/or longitude using collapse. Only possible if the dataset contains latitude and longitude coordinates and for regular grids. Must be one of 'land', 'sea'.

# mask: dict of dict

Mask datasets. Keys have to be numpy.ma conversion operations (see https://docs.scipy.org/doc/numpy/ reference/routines.ma.html) and values all the keyword arguments of them.

# n\_jobs: int (default: 1)

Maximum number of jobs spawned by this diagnostic script. Use -1 to use all processors. More details are given here.

#### normalize\_by\_mean: bool, optional (default: False)

Remove total mean of the dataset in the last step (resulting mean will be 0.0). Calculates weighted mean if area\_weighted, time\_weighted or landsea\_fraction\_weighted are set and the cube contains the corresponding coordinates. Does not apply to error datasets.

# normalize\_by\_std: bool, optional (default: False)

Scale total standard deviation of the dataset in the last step (resulting standard deviation will be 1.0).

# output\_attributes: dict, optional

Write additional attributes to netcdf files, e.g. 'tag'.

#### pattern: str, optional

Pattern matched against ancestor file names.

#### ref\_calculation: str, optional

Perform calculations involving reference dataset. Must be one of merge (simply merge two datasets by adding the data of the reference dataset as iris.coords.AuxCoord to the original dataset), add (add reference dataset), divide (divide by reference dataset), multiply (multiply with reference dataset), subtract (subtract reference dataset) or trend (use reference dataset as x axis for calculation of linear trend along a specified axis, see ref\_kwargs).

#### ref\_kwargs: dict, optional

Keyword arguments for calculations involving reference datasets. Allowed keyword arguments are:

- matched\_by (list of str, default: []): Use a given set of attributes to match datasets with their corresponding reference datasets (specified by ref = True).
- collapse\_over (str, default: 'time'): Coordinate which is collapsed. Only relevant when ref\_calculation is set to trend.

#### return\_trend\_stderr: bool, optional (default: True)

Return standard error of slope in case of trend calculations (as var\_type prediction\_input\_error).

# scalar\_operations: dict, optional

Operations involving scalars. Allowed keys are add, divide, multiply or subtract. The corresponding values (float or int) are scalars that are used with the operations.

# time\_weighted: bool, optional (default: True)

Use weighted aggregation when collapsing over time dimension using collapse. Weights are estimated using time bounds.

# unify\_coords\_to: dict, optional

If given, replace coordinates of all datasets with that of a reference cube (if necessary and possible, broadcast beforehand). The reference dataset is determined by keyword arguments given to this option (keyword arguments must point to exactly one dataset).

# **Rescale data with emergent constraints**

Rescale label data using a single emergent constraint.

# Description

This diagnostic uses an emergent relationship between data marked as var\_type=label (Y axis) and var\_type=feature (X axis) together with an observation of the X axis (var\_type=prediction\_input and var\_type=prediction\_input\_error) to calculate factors that are necessary to rescale each input point so that it matches the constraint. The rescaling is applied to data marked as var\_type=label\_to\_rescale. All data needs the attribute tag which needs to be identical for label, prediction\_input, prediction\_input\_error and label\_to\_rescale. Only a single tag for feature is possible.

# Author

Manuel Schlund (DLR, Germany)

# Project

CRESCENDO

# **Configuration options in recipe**

# group\_by\_attributes: list of str, optional (default: ['dataset'])

List of attributes used to separate different input points.

# ignore: list of dict, optional

Ignore specific datasets by specifying multiple dict s of metadata.

#### legend\_kwargs: dict, optional

Optional keyword arguments of matplotlib.pyplot.legend() (affects only plots with legends).

#### pattern: str, optional

Pattern matched against ancestor file names.

#### plot\_emergent\_relationship: dict, optional

If given, plot emergent relationship between X and Y data. Specify additional keyword arguments by plot\_kwargs and plot appearance options by pyplot\_kwargs (processed as functions of matplotlib. pyplot). Use {} to plot with default settings.

#### plot\_kwargs\_for\_groups: dict, optional

Specify additional keyword arguments (values) for the different points defined by group\_by\_attributes (keys) used in plots.

# savefig\_kwargs: dict, optional

Keyword arguments for matplotlib.pyplot.savefig().

#### seaborn\_settings: dict, optional

Options for seaborn.set\_theme() (affects all plots).

# 54.2.3 Auxiliary scripts

#### Auxiliary functions for MLR scripts

Convenience functions for MLR diagnostics.

# **Functions:**

<pre>check_predict_kwargs(predict_kwargs)</pre>	Check keyword argument for predict() functions.
create_alias(dataset, attributes[, delimiter])	Create alias key of a dataset using a list of attributes.
<pre>datasets_have_mlr_attributes(datasets[,])</pre>	Check (MLR) attributes of datasets.
<pre>get_1d_cube(x_data, y_data[, x_kwargs, y_kwargs])</pre>	Convert 2 arrays to iris.cube.Cube (with single coordinate).
<pre>get_absolute_time_units(units)</pre>	Convert time reference units to absolute ones.
get_alias(dataset)	Get alias for dataset.
<pre>get_all_weights(cube[, area_weighted,])</pre>	Get all desired weights for a cube.
<pre>get_area_weights(cube[, normalize])</pre>	Get area weights calculated from grid cell areas.
<pre>get_horizontal_weights(cube[,])</pre>	Get horizontal (latitude/longitude) weights of cube.
<pre>get_input_data(cfg[, pattern,])</pre>	Get input data and check MLR attributes if desired.
<pre>get_landsea_fraction_weights(cube, area_type)</pre>	Get land/sea fraction weights calculated from Natural Earth files.
<pre>get_new_path(cfg, old_path)</pre>	Convert old path to new diagnostic path.
<pre>get_squared_error_cube(ref_cube, error_datasets)</pre>	Get array of squared errors.
<pre>get_time_weights(cube[, normalize])</pre>	Get time weights of cube calculated from time bounds.
ignore_warnings()	Ignore warnings given by WARNINGS_TO_IGNORE.
<pre>square_root_metadata(cube)</pre>	Take the square root of the cube metadata.
<pre>units_power(units, power)</pre>	Raise a cf_units.Unit to given power preserving symbols.

esmvaltool.diag\_scripts.mlr.check\_predict\_kwargs(predict\_kwargs)

Check keyword argument for predict() functions.

# Parameters

predict\_kwargs (keyword arguments, optional) - Keyword arguments for a
predict() function.

#### Raises

**RuntimeError** – return\_var and return\_cov are both set to True in the keyword arguments.

# esmvaltool.diag\_scripts.mlr.create\_alias(dataset, attributes, delimiter='-')

Create alias key of a dataset using a list of attributes.

#### **Parameters**

• **dataset** (*dict*) – Metadata dictionary representing a single dataset.

- attributes (list of str) List of attributes used to create the alias.
- **delimiter** (*str*, *optional* (*default:* '-')) Delimiter used to separate different attributes in the alias.

#### Returns

Dataset alias.

# **Return type**

str

#### Raises

AttributeError – dataset does not contain one of the attributes.

esmvaltool.diag\_scripts.mlr.datasets\_have\_mlr\_attributes(*datasets*, *log\_level='debug'*, *mode='full'*) Check (MLR) attributes of datasets.

## Parameters

- datasets (list of dict) Datasets to check.
- log\_level (str, optional (default: 'debug')) Verbosity level of the logger.
- mode (str, optional (default: 'full')) Checking mode. Must be one of 'only\_missing' (only check if attributes are missing), 'only\_var\_type' (check only var\_type) or 'full' (check both).

#### Returns

True if all required attributes are available, False if not.

#### **Return type**

bool

# Raises

ValueError – Invalid value for argument mode is given.

esmvaltool.diag\_scripts.mlr.get\_1d\_cube(x\_data, y\_data, x\_kwargs=None, y\_kwargs=None)
Convert 2 arrays to iris.cube.Cube (with single coordinate).

#### **Parameters**

- **x\_data** (*numpy.ndarray*) Data for coordinate.
- **y\_data** (*numpy.ndarray*) Data for cube.
- **x\_kwargs** (*dict*) Keyword arguments passed to iris.coords.AuxCoord.
- y\_kwargs (dict) Keyword arguments passed to iris.cube.Cube.

#### Returns

1D cube with single auxiliary coordinate.

#### **Return type**

iris.cube.Cube

#### Raises

ValueError – Arrays are not 1D and do not have matching shapes.

#### esmvaltool.diag\_scripts.mlr.get\_absolute\_time\_units(units)

Convert time reference units to absolute ones.

This function converts reference time units (like 'days since YYYY') to absolute ones (like 'days').

#### **Parameters**

units (cf\_units.Unit) - Time units to convert.

#### Returns

Absolute time units.

#### **Return type**

cf\_units.Unit

# Raises

ValueError – If conversion failed (e.g. input units are not time units).

esmvaltool.diag\_scripts.mlr.get\_alias(dataset)

Get alias for dataset.

Parameters

dataset (dict) – Dataset metadata.

Returns

Alias.

#### **Return type**

str

Get all desired weights for a cube.

# Parameters

- cube (*iris.cube.Cube*) Input cube.
- area\_weighted (bool, optional (default: True)) Use area weights calculated from grid cell areas using iris.analysis.cartography.area\_weights(). Only works for regular grids.
- **time\_weighted** (*bool*, *optional* (*default: True*)) Use time weights calculated from time bounds.
- landsea\_fraction\_weighted (*str*, *optional*) If given, use land/sea fraction weights calculated from Natural Earth files. Must be one of 'land', 'sea'. Only works for regular grids.
- **normalize** (*bool*, *optional* (*default: False*)) Normalize weights with total area and total time range.

#### Returns

Area weights.

#### **Return type**

numpy.ndarray

#### Raises

- iris.exceptions.CoordinateMultiDimError Dimension of latitude or longitude coordinate is greater than 1.
- **iris.exceptions.CoordinateNotFoundError** Cube does not contain the coordinates latitude and longitude (if used with area\_weighted or landsea\_fraction\_weighted) or cube does not contain the coordinate time (if used with time\_weighted).
- ValueError landsea\_fraction\_weighted is not one of None, 'land', 'sea' or coordinates latitude and longitude share dimensions.

#### esmvaltool.diag\_scripts.mlr.get\_area\_weights(cube, normalize=False)

Get area weights calculated from grid cell areas.

**Note:** Only works for regular grids. Uses iris.analysis.cartography.area\_weights() for an approximate calculation of the grid cell areas.

#### Parameters

- cube (iris.cube.Cube) Input cube.
- **normalize** (*bool*, *optional* (*default: False*)) Normalize weights with total area.

#### Returns

Area weights.

#### **Return type**

numpy.ndarray

# Raises

**iris.exceptions.CoordinateNotFoundError** – Cube does not contain the coordinates latitude and longitude.

Get horizontal (latitude/longitude) weights of cube.

#### **Parameters**

- **cube** (*iris.cube.Cube*) Input cube.
- area\_weighted (bool, optional (default: True)) Use area weights calculated from grid cell areas using iris.analysis.cartography.area\_weights(). Only works for regular grids.
- landsea\_fraction\_weighted (*str*, *optional*) If given, use land/sea fraction weights calculated from Natural Earth files. Must be one of 'land', 'sea'. Only works for regular grids.
- **normalize** (*bool*, *optional* (*default: False*)) Normalize weights with sum of weights over latitude and longitude (i.e. if only area\_weighted is given, this is equal to the total area).

# Returns

Horizontal (latitude/longitude) weights.

#### **Return type**

numpy.ndarray

#### Raises

- iris.exceptions.CoordinateMultiDimError Dimension of latitude or longitude coordinate is greater than 1.
- iris.exceptions.CoordinateNotFoundError Cube does not contain the coordinates latitude and longitude.
- ValueError landsea\_fraction\_weighted is not one of 'land', 'sea'.

Get input data and check MLR attributes if desired.

Use input\_data and ancestors to get all relevant input files.

#### **Parameters**

- **cfg** (*dict*) Recipe configuration.
- pattern (str, optional) Pattern matched against ancestor file names.
- **check\_mlr\_attributes** (*bool*, *optional* (*default: True*)) If True, only returns datasets with valid MLR attributes. If False, returns all found datasets.
- **ignore** (*list of dict, optional*) Ignore specific datasets by specifying multiple dict`s of metadata. By setting an attribute to ``None`, ignore all datasets which do not have that attribute.

#### Returns

List of input datasets.

#### **Return type**

list of dict

## Raises

**ValueError** – No input data found or at least one dataset has invalid attributes.

esmvaltool.diag\_scripts.mlr.get\_landsea\_fraction\_weights(cube, area\_type, normalize=False)

Get land/sea fraction weights calculated from Natural Earth files.

**Note:** The implementation of this feature is not optimal. For large cubes, calculating the land/sea fraction weights might be very slow. Only works for regular grids.

#### Parameters

- cube (iris.cube.Cube) Input cube.
- **area\_type** (*str*) Area type. Must be one of 'land' (land fraction weighting) or 'sea' (sea fraction weighting).
- **normalize** (*bool*, *optional* (*default: False*)) Normalize weights with total land/sea fraction.

# Raises

- iris.exceptions.CoordinateMultiDimError Dimension of latitude or longitude coordinate is greater than 1.
- iris.exceptions.CoordinateNotFoundError Cube does not contain the coordinates latitude and longitude.
- ValueError area\_type is not one of 'land', 'sea' or coordinates latitude and longitude share dimensions.

#### esmvaltool.diag\_scripts.mlr.get\_new\_path(cfg, old\_path)

Convert old path to new diagnostic path.

# Parameters

• **cfg** (*dict*) – Recipe configuration.

• old\_path (str) – Old path.

# Returns

New diagnostic path.

# Return type

str

esmvaltool.diag\_scripts.mlr.get\_squared\_error\_cube(ref\_cube, error\_datasets)

Get array of squared errors.

#### **Parameters**

- **ref\_cube** (*iris.cube.Cube*) Reference cube (determines mask, coordinates and attributes of output).
- **error\_datasets** (*list of dict*) List of metadata dictionaries where each dictionary represents a single dataset.

#### Returns

Cube containing squared errors.

#### **Return type**

iris.cube.Cube

# Raises

ValueError – Shape of a dataset does not match shape of reference cube.

esmvaltool.diag\_scripts.mlr.get\_time\_weights(cube, normalize=False)

Get time weights of cube calculated from time bounds.

#### **Parameters**

- cube (iris.cube.Cube) Input cube.
- **normalize** (*bool*, *optional* (*default: False*)) Normalize weights with total time range.

#### Returns

Time weights.

#### **Return type**

numpy.ndarray

#### Raises

iris.exceptions.CoordinateNotFoundError - Cube does not contain the coordinate
time.

#### esmvaltool.diag\_scripts.mlr.ignore\_warnings()

Ignore warnings given by WARNINGS\_TO\_IGNORE.

# esmvaltool.diag\_scripts.mlr.square\_root\_metadata(cube)

Take the square root of the cube metadata.

#### Parameters

cube (*iris.cube.Cube*) – Cube (will be modified in-place).

#### esmvaltool.diag\_scripts.mlr.units\_power(units, power)

Raise a cf\_units.Unit to given power preserving symbols.

Raise cf\_units.Unit to given power without expanding it first. For example, using units\_power(Unit('J'), 2) gives Unit('J2'). In contrast, simply using Unit('J')\*\*2 would yield 'kg2 m4 s-4'.

# Parameters

- **units** (*cf\_units.Unit*) Input units.
- **power** (*int*) Desired exponent.

# Returns

Input units raised to given power.

# **Return type**

cf\_units.Unit

# Raises

- **TypeError** Argument **power** is not int-like.
- ValueError Invalid unit given.

# Custom extensions of sklearn functionalities

Custom expansions of sklearn functionalities.

**Note:** This module provides custom expansions of some sklearn classes and functions which are necessary to fit the purposes for the desired functionalities of the *MLR module*. As long-term goal we would like to include these functionalities to the sklearn package since we believe these additions might be helpful for everyone. This module serves as interim solution. To ensure that all features are properly working this module is also covered by extensive tests.

Parts of this code have been copied from sklearn.

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#### Bases: Pipeline

Expand sklearn.pipeline.Pipeline.

# property classes\_

The classes labels. Only exist if the last step is a classifier.

# property coef\_

Model coefficients.

Туре

numpy.ndarray

#### **decision\_function**(*X*, \*\**params*)

Transform the data, and apply *decision\_function* with the final estimator.

Call *transform* of each transformer in the pipeline. The transformed data are finally passed to the final estimator that calls *decision\_function* method. Only valid if the final estimator implements *decision\_function*.

#### **Parameters**

- **X** (*iterable*) Data to predict on. Must fulfill input requirements of first step of the pipeline.
- \*\*params (dict of string -> object) Parameters requested and accepted by steps. Each step must have requested certain metadata for these parameters to be forwarded to them.

Added in version 1.4: Only available if *enable\_metadata\_routing=True*. See Metadata Routing User Guide for more details.

#### Returns

y\_score – Result of calling *decision\_function* on the final estimator.

#### **Return type**

ndarray of shape (n\_samples, n\_classes)

# property feature\_importances\_

Feature importances.

Туре

numpy.ndarray

#### property feature\_names\_in\_

Names of features seen during first step fit method.

# fit(X, y=None, \*\*params)

Fit the model.

Fit all the transformers one after the other and sequentially transform the data. Finally, fit the transformed data using the final estimator.

# **Parameters**

- **X** (*iterable*) Training data. Must fulfill input requirements of first step of the pipeline.
- **y** (*iterable*, *default=None*) Training targets. Must fulfill label requirements for all steps of the pipeline.
- **\*\*params** (dict of str -> object) -
  - If enable\_metadata\_routing=False (default):

Parameters passed to the fit method of each step, where each parameter name is prefixed such that parameter p for step s has key s\_\_p.

- If enable\_metadata\_routing=True:

Parameters requested and accepted by steps. Each step must have requested certain metadata for these parameters to be forwarded to them.

Changed in version 1.4: Parameters are now passed to the transform method of the intermediate steps as well, if requested, and if *enable\_metadata\_routing=True* is set via set\_config().

See Metadata Routing User Guide for more details.

Returns

**self** – Pipeline with fitted steps.

Return type object

fit\_predict(X, y=None, \*\*params)

Transform the data, and apply *fit\_predict* with the final estimator.

Call *fit\_transform* of each transformer in the pipeline. The transformed data are finally passed to the final estimator that calls *fit\_predict* method. Only valid if the final estimator implements *fit\_predict*.

#### **Parameters**

- **X** (*iterable*) Training data. Must fulfill input requirements of first step of the pipeline.
- **y** (*iterable*, *default=None*) Training targets. Must fulfill label requirements for all steps of the pipeline.
- **\*\*params** (dict of str -> object) -
  - If enable\_metadata\_routing=False (default):

Parameters to the predict called at the end of all transformations in the pipeline.

- If enable\_metadata\_routing=True:

Parameters requested and accepted by steps. Each step must have requested certain metadata for these parameters to be forwarded to them.

Added in version 0.20.

Changed in version 1.4: Parameters are now passed to the transform method of the intermediate steps as well, if requested, and if *enable\_metadata\_routing=True*.

See Metadata Routing User Guide for more details.

Note that while this may be used to return uncertainties from some models with return\_std or return\_cov, uncertainties that are generated by the transformations in the pipeline are not propagated to the final estimator.

## Returns

**y\_pred** – Result of calling *fit\_predict* on the final estimator.

#### **Return type**

ndarray

# fit\_target\_transformer\_only(y\_data, \*\*fit\_kwargs)

Fit only transform step of of target regressor.

# fit\_transform(X, y=None, \*\*params)

Fit the model and transform with the final estimator.

Fit all the transformers one after the other and sequentially transform the data. Only valid if the final estimator either implements *fit\_transform* or *fit* and *transform*.

#### Parameters

- **X** (*iterable*) Training data. Must fulfill input requirements of first step of the pipeline.
- **y** (*iterable*, *default=None*) Training targets. Must fulfill label requirements for all steps of the pipeline.
- **\*\*params** (dict of str -> object) -
  - If enable\_metadata\_routing=False (default):

Parameters passed to the fit method of each step, where each parameter name is prefixed such that parameter p for step s has key s\_\_p.

- If enable\_metadata\_routing=True:

Parameters requested and accepted by steps. Each step must have requested certain metadata for these parameters to be forwarded to them.

Changed in version 1.4: Parameters are now passed to the transform method of the intermediate steps as well, if requested, and if *enable\_metadata\_routing=True*.

See Metadata Routing User Guide for more details.

#### Returns

**Xt** – Transformed samples.

#### **Return type**

ndarray of shape (n\_samples, n\_transformed\_features)

#### fit\_transformers\_only(x\_data, y\_data, \*\*fit\_kwargs)

Fit only transform steps of Pipeline.

#### get\_feature\_names\_out(input\_features=None)

Get output feature names for transformation.

Transform input features using the pipeline.

#### Parameters

input\_features (array-like of str or None, default=None) - Input features.

#### Returns

feature\_names\_out – Transformed feature names.

# **Return type**

ndarray of str objects

#### get\_metadata\_routing()

Get metadata routing of this object.

Please check User Guide on how the routing mechanism works.

#### Returns

routing – A MetadataRouter encapsulating routing information.

#### **Return type**

MetadataRouter

## get\_params(deep=True)

Get parameters for this estimator.

Returns the parameters given in the constructor as well as the estimators contained within the *steps* of the *Pipeline*.

#### **Parameters**

**deep** (*bool*, *default=True*) – If True, will return the parameters for this estimator and contained subobjects that are estimators.

#### Returns

params – Parameter names mapped to their values.

# Return type

mapping of string to any

# inverse\_transform(Xt, \*\*params)

Apply *inverse\_transform* for each step in a reverse order.

All estimators in the pipeline must support *inverse\_transform*.

#### **Parameters**

- Xt (array-like of shape (n\_samples, n\_transformed\_features)) Data samples, where n\_samples is the number of samples and n\_features is the number of features. Must fulfill input requirements of last step of pipeline's inverse\_transform method.
- **\*\*params** (*dict of str -> object*) Parameters requested and accepted by steps. Each step must have requested certain metadata for these parameters to be forwarded to them.

Added in version 1.4: Only available if *enable\_metadata\_routing=True*. See Metadata Routing User Guide for more details.

# Returns

**Xt** – Inverse transformed data, that is, data in the original feature space.

#### **Return type**

ndarray of shape (n\_samples, n\_features)

# property n\_features\_in\_

Number of features seen during first step fit method.

#### property named\_steps

Access the steps by name.

Read-only attribute to access any step by given name. Keys are steps names and values are the steps objects.

#### predict(X, \*\*params)

Transform the data, and apply *predict* with the final estimator.

Call *transform* of each transformer in the pipeline. The transformed data are finally passed to the final estimator that calls *predict* method. Only valid if the final estimator implements *predict*.

#### **Parameters**

• **X** (*iterable*) – Data to predict on. Must fulfill input requirements of first step of the pipeline.

- **\*\*params**(dict of str -> object)-
  - If enable\_metadata\_routing=False (default):

Parameters to the **predict** called at the end of all transformations in the pipeline.

- If enable\_metadata\_routing=True:

Parameters requested and accepted by steps. Each step must have requested certain metadata for these parameters to be forwarded to them.

#### Added in version 0.20.

Changed in version 1.4: Parameters are now passed to the transform method of the intermediate steps as well, if requested, and if *enable\_metadata\_routing=True* is set via set\_config().

See Metadata Routing User Guide for more details.

Note that while this may be used to return uncertainties from some models with return\_std or return\_cov, uncertainties that are generated by the transformations in the pipeline are not propagated to the final estimator.

#### Returns

y\_pred – Result of calling *predict* on the final estimator.

# Return type

ndarray

#### predict\_log\_proba(X, \*\*params)

Transform the data, and apply *predict\_log\_proba* with the final estimator.

Call *transform* of each transformer in the pipeline. The transformed data are finally passed to the final estimator that calls *predict\_log\_proba* method. Only valid if the final estimator implements *predict\_log\_proba*.

# Parameters

- **X** (*iterable*) Data to predict on. Must fulfill input requirements of first step of the pipeline.
- **\*\*params** (dict of str -> object) -
  - If enable\_metadata\_routing=False (default):

Parameters to the *predict\_log\_proba* called at the end of all transformations in the pipeline.

- If enable\_metadata\_routing=True:

Parameters requested and accepted by steps. Each step must have requested certain metadata for these parameters to be forwarded to them.

Added in version 0.20.

Changed in version 1.4: Parameters are now passed to the transform method of the intermediate steps as well, if requested, and if *enable\_metadata\_routing=True*.

See Metadata Routing User Guide for more details.

#### Returns

y\_log\_proba – Result of calling *predict\_log\_proba* on the final estimator.

#### **Return type**

ndarray of shape (n\_samples, n\_classes)

#### predict\_proba(X, \*\*params)

Transform the data, and apply *predict\_proba* with the final estimator.

Call *transform* of each transformer in the pipeline. The transformed data are finally passed to the final estimator that calls *predict\_proba* method. Only valid if the final estimator implements *predict\_proba*.

#### Parameters

- **X** (*iterable*) Data to predict on. Must fulfill input requirements of first step of the pipeline.
- **\*\*params**(dict of str -> object)-
  - If enable\_metadata\_routing=False (default):

Parameters to the *predict\_proba* called at the end of all transformations in the pipeline.

- If enable\_metadata\_routing=True:

Parameters requested and accepted by steps. Each step must have requested certain metadata for these parameters to be forwarded to them.

Added in version 0.20.

Changed in version 1.4: Parameters are now passed to the transform method of the intermediate steps as well, if requested, and if *enable\_metadata\_routing=True*.

See Metadata Routing User Guide for more details.

#### Returns

y\_proba – Result of calling *predict\_proba* on the final estimator.

#### Return type

ndarray of shape (n\_samples, n\_classes)

## score(X, y=None, sample\_weight=None, \*\*params)

Transform the data, and apply *score* with the final estimator.

Call *transform* of each transformer in the pipeline. The transformed data are finally passed to the final estimator that calls *score* method. Only valid if the final estimator implements *score*.

#### **Parameters**

- **X** (*iterable*) Data to predict on. Must fulfill input requirements of first step of the pipeline.
- **y** (*iterable*, *default=None*) Targets used for scoring. Must fulfill label requirements for all steps of the pipeline.
- **sample\_weight** (*array-like*, *default=None*) If not None, this argument is passed as sample\_weight keyword argument to the score method of the final estimator.
- **\*\*params** (dict of str -> object) Parameters requested and accepted by steps. Each step must have requested certain metadata for these parameters to be forwarded to them.

Added in version 1.4: Only available if *enable\_metadata\_routing=True*. See Metadata Routing User Guide for more details.

#### Returns

score – Result of calling score on the final estimator.

#### **Return type**

float

# score\_samples(X)

Transform the data, and apply *score\_samples* with the final estimator.

Call *transform* of each transformer in the pipeline. The transformed data are finally passed to the final estimator that calls *score\_samples* method. Only valid if the final estimator implements *score\_samples*.

#### **Parameters**

 $\mathbf{X}$  (*iterable*) – Data to predict on. Must fulfill input requirements of first step of the pipeline.

#### Returns

y\_score – Result of calling *score\_samples* on the final estimator.

#### **Return type**

ndarray of shape (n\_samples,)

#### set\_output(\*, transform=None)

Set the output container when "transform" and "fit\_transform" are called.

Calling set\_output will set the output of all estimators in steps.

#### **Parameters**

**transform** ({"default", "pandas"}, default=None) – Configure output of *transform* and *fit\_transform*.

- "default": Default output format of a transformer
- "pandas": DataFrame output
- "polars": Polars output
- None: Transform configuration is unchanged

Added in version 1.4: "polars" option was added.

# Returns

self – Estimator instance.

# Return type

estimator instance

#### set\_params(\*\*kwargs)

Set the parameters of this estimator.

Valid parameter keys can be listed with get\_params(). Note that you can directly set the parameters of the estimators contained in *steps*.

# Parameters

**\*\*kwargs** (*dict*) – Parameters of this estimator or parameters of estimators contained in *steps*. Parameters of the steps may be set using its name and the parameter name separated by a '\_\_'.

# Returns

self – Pipeline class instance.

# **Return type**

object

set\_score\_request(\*, sample\_weight: bool | None | str ='\$UNCHANGED\$')  $\rightarrow$  AdvancedPipeline Request metadata passed to the score method.

Note that this method is only relevant if enable\_metadata\_routing=True (see sklearn. set\_config()). Please see User Guide on how the routing mechanism works.

The options for each parameter are:

- True: metadata is requested, and passed to score if provided. The request is ignored if metadata is not provided.
- False: metadata is not requested and the meta-estimator will not pass it to score.
- None: metadata is not requested, and the meta-estimator will raise an error if the user provides it.
- str: metadata should be passed to the meta-estimator with this given alias instead of the original name.

The default (sklearn.utils.metadata\_routing.UNCHANGED) retains the existing request. This allows you to change the request for some parameters and not others.

Added in version 1.3.

**Note:** This method is only relevant if this estimator is used as a sub-estimator of a meta-estimator, e.g. used inside a Pipeline. Otherwise it has no effect.

#### **Parameters**

sample\_weight (str, True, False, or None, default=sklearn.utils. metadata\_routing.UNCHANGED) - Metadata routing for sample\_weight parameter in score.

# Returns

self - The updated object.

# Return type object

#### steps: List[Any]

#### **transform**(*X*, \*\**params*)

Transform the data, and apply *transform* with the final estimator.

Call *transform* of each transformer in the pipeline. The transformed data are finally passed to the final estimator that calls *transform* method. Only valid if the final estimator implements *transform*.

This also works where final estimator is None in which case all prior transformations are applied.

#### Parameters

- **X** (*iterable*) Data to transform. Must fulfill input requirements of first step of the pipeline.
- **\*\*params** (*dict of str -> object*) Parameters requested and accepted by steps. Each step must have requested certain metadata for these parameters to be forwarded to them.

Added in version 1.4: Only available if *enable\_metadata\_routing=True*. See Metadata Routing User Guide for more details.

#### Returns

Xt – Transformed data.

#### **Return type**

ndarray of shape (n\_samples, n\_transformed\_features)

# transform\_only(x\_data)

Only perform transform steps of Pipeline.

# transform\_target\_only(y\_data)

Only perform transform steps of target regressor.

class esmvaltool.diag\_scripts.mlr.custom\_sklearn.AdvancedRFE(estimator, \*,

n\_features\_to\_select=None, step=1, verbose=0, importance\_getter='auto')

Bases: RFE

Expand sklearn.feature\_selection.RFE.

# property classes\_

Classes labels available when estimator is a classifier.

#### Return type

ndarray of shape (n\_classes,)

# decision\_function(X)

Compute the decision function of X.

#### **Parameters**

**X** ({array-like or sparse matrix} of shape (n\_samples, n\_features)) – The input samples. Internally, it will be converted to dtype=np.float32 and if a sparse matrix is provided to a sparse csr\_matrix.

#### Returns

score – The decision function of the input samples. The order of the classes corresponds to that in the attribute classes\_. Regression and binary classification produce an array of shape [n\_samples].

#### **Return type**

array, shape = [n\_samples, n\_classes] or [n\_samples]

#### fit(x\_data, y\_data, \*\*fit\_kwargs)

Expand fit() to accept kwargs.

# fit\_transform(X, y=None, \*\*fit\_params)

Fit to data, then transform it.

Fits transformer to X and y with optional parameters *fit\_params* and returns a transformed version of X.

# **Parameters**

- X (array-like of shape (n\_samples, n\_features)) Input samples.
- **y** (array-like of shape (n\_samples,) or (n\_samples, n\_outputs), default=None) Target values (None for unsupervised transformations).
- **\*\*fit\_params** (*dict*) Additional fit parameters.

#### Returns

**X\_new** – Transformed array.

# **Return type**

ndarray array of shape (n\_samples, n\_features\_new)

#### get\_feature\_names\_out(input\_features=None)

Mask feature names according to selected features.

# Parameters

**input\_features** (array-like of str or None, default=None) – Input features.

- If *input\_features* is *None*, then *feature\_names\_in\_* is used as feature names in. If *feature\_names\_in\_* is not defined, then the following input feature names are generated: ["x0", "x1", ..., "x(n\_features\_in\_ 1)"].
- If *input\_features* is an array-like, then *input\_features* must match *feature\_names\_in\_* if *feature\_names\_in\_* is defined.

#### Returns

feature\_names\_out – Transformed feature names.

#### **Return type**

ndarray of str objects

#### get\_metadata\_routing()

Raise NotImplementedError.

This estimator does not support metadata routing yet.

#### get\_params(deep=True)

Get parameters for this estimator.

#### **Parameters**

**deep** (*bool*, *default=True*) – If True, will return the parameters for this estimator and contained subobjects that are estimators.

#### Returns

params – Parameter names mapped to their values.

**Return type** 

dict

# get\_support(indices=False)

Get a mask, or integer index, of the features selected.

#### Parameters

**indices** (*bool*, *default=False*) – If True, the return value will be an array of integers, rather than a boolean mask.

#### Returns

**support** – An index that selects the retained features from a feature vector. If *indices* is False, this is a boolean array of shape [# input features], in which an element is True iff its corresponding feature is selected for retention. If *indices* is True, this is an integer array of shape [# output features] whose values are indices into the input feature vector.

#### **Return type**

array

# inverse\_transform(X)

Reverse the transformation operation.

#### Parameters

**X** (array of shape [n\_samples, n\_selected\_features]) – The input samples.

#### Returns

 $X_r - X$  with columns of zeros inserted where features would have been removed by *transform()*.

#### **Return type**

array of shape [n\_samples, n\_original\_features]

predict(x\_data, \*\*predict\_kwargs)

Expand predict () to accept kwargs.

## predict\_log\_proba(X)

Predict class log-probabilities for X.

#### Parameters

X (array of shape [n\_samples, n\_features]) – The input samples.

#### Returns

 $\mathbf{p}$  – The class log-probabilities of the input samples. The order of the classes corresponds to that in the attribute classes\_.

# **Return type**

array of shape (n\_samples, n\_classes)

# predict\_proba(X)

Predict class probabilities for X.

#### Parameters

**X** ({array-like or sparse matrix} of shape (n\_samples, n\_features)) – The input samples. Internally, it will be converted to dtype=np.float32 and if a sparse matrix is provided to a sparse csr\_matrix.

# Returns

 $\mathbf{p}$  – The class probabilities of the input samples. The order of the classes corresponds to that in the attribute classes\_.

#### **Return type**

array of shape (n\_samples, n\_classes)

# score(X, y, \*\*fit\_params)

Reduce X to the selected features and return the score of the estimator.

# Parameters

- X (array of shape [n\_samples, n\_features]) The input samples.
- y (array of shape [n\_samples]) The target values.
- **\*\*fit\_params** (*dict*) Parameters to pass to the *score* method of the underlying estimator.

Added in version 1.0.

#### Returns

**score** – Score of the underlying base estimator computed with the selected features returned by *rfe.transform*(X) and y.

# **Return type**

float

```
set_fit_request(*, x_data: bool | None | str = '$UNCHANGED$', y_data: bool | None | str = '$UNCHANGED$') \rightarrow AdvancedRFE
```

Request metadata passed to the fit method.

Note that this method is only relevant if enable\_metadata\_routing=True (see sklearn. set\_config()). Please see User Guide on how the routing mechanism works.

The options for each parameter are:

- True: metadata is requested, and passed to fit if provided. The request is ignored if metadata is not provided.
- False: metadata is not requested and the meta-estimator will not pass it to fit.
- None: metadata is not requested, and the meta-estimator will raise an error if the user provides it.
- str: metadata should be passed to the meta-estimator with this given alias instead of the original name.

The default (sklearn.utils.metadata\_routing.UNCHANGED) retains the existing request. This allows you to change the request for some parameters and not others.

Added in version 1.3.

**Note:** This method is only relevant if this estimator is used as a sub-estimator of a meta-estimator, e.g. used inside a Pipeline. Otherwise it has no effect.

#### **Parameters**

- **x\_data** (str, True, False, or None, default=sklearn.utils. metadata\_routing.UNCHANGED) - Metadata routing for x\_data parameter in fit.
- y\_data (str, True, False, or None, default=sklearn.utils. metadata\_routing.UNCHANGED) Metadata routing for y\_data parameter in fit.

#### Returns

self – The updated object.

**Return type** 

object

# set\_output(\*, transform=None)

Set output container.

See Introducing the set\_output API for an example on how to use the API.

#### **Parameters**

**transform** ({"default", "pandas"}, default=None) – Configure output of *transform* and *fit\_transform*.

- "default": Default output format of a transformer
- "pandas": DataFrame output
- "polars": Polars output
- None: Transform configuration is unchanged

Added in version 1.4: "polars" option was added.

#### Returns

self – Estimator instance.

#### **Return type**

estimator instance

#### set\_params(\*\*params)

Set the parameters of this estimator.

The method works on simple estimators as well as on nested objects (such as Pipeline). The latter have parameters of the form <component>\_\_<parameter> so that it's possible to update each component of a nested object.

#### **Parameters**

**\*\*params** (*dict*) – Estimator parameters.

Returns

**self** – Estimator instance.

# Return type

estimator instance

 $set_predict_request(*, x_data: bool | None | str = '$UNCHANGED$') \rightarrow AdvancedRFE$ 

Request metadata passed to the predict method.

Note that this method is only relevant if enable\_metadata\_routing=True (see sklearn. set\_config()). Please see User Guide on how the routing mechanism works.

The options for each parameter are:

- True: metadata is requested, and passed to predict if provided. The request is ignored if metadata is not provided.
- False: metadata is not requested and the meta-estimator will not pass it to predict.
- None: metadata is not requested, and the meta-estimator will raise an error if the user provides it.
- str: metadata should be passed to the meta-estimator with this given alias instead of the original name.

The default (sklearn.utils.metadata\_routing.UNCHANGED) retains the existing request. This allows you to change the request for some parameters and not others.

Added in version 1.3.

**Note:** This method is only relevant if this estimator is used as a sub-estimator of a meta-estimator, e.g. used inside a Pipeline. Otherwise it has no effect.

# Parameters

x\_data (str, True, False, or None, default=sklearn.utils. metadata\_routing.UNCHANGED) - Metadata routing for x\_data parameter in predict.

Returns

self – The updated object.

**Return type** 

object

#### transform(X)

Reduce X to the selected features.

# Parameters

**X**(array of shape [n\_samples, n\_features]) – The input samples.

#### Returns

 $X_r$  – The input samples with only the selected features.

# **Return type**

array of shape [n\_samples, n\_selected\_features]

class esmvaltool.diag\_scripts.mlr.custom\_sklearn.AdvancedRFECV(estimator, step=1,

min\_features\_to\_select=1, cv=None, scoring=None, verbose=0, n\_jobs=None)

Bases: AdvancedRFE

Expand sklearn.feature\_selection.RFECV.

#### property classes\_

Classes labels available when estimator is a classifier.

# **Return type**

ndarray of shape (n\_classes,)

# decision\_function(X)

Compute the decision function of X.

#### **Parameters**

**X** ({array-like or sparse matrix} of shape (n\_samples, n\_features)) – The input samples. Internally, it will be converted to dtype=np.float32 and if a sparse matrix is provided to a sparse csr\_matrix.

#### Returns

**score** – The decision function of the input samples. The order of the classes corresponds to that in the attribute classes\_. Regression and binary classification produce an array of shape [n\_samples].

# **Return type**

array, shape = [n\_samples, n\_classes] or [n\_samples]

#### **fit**(*x\_data*, *y\_data*, *groups=None*, \*\**fit\_kwargs*)

Expand fit() to accept kwargs.

# fit\_transform(X, y=None, \*\*fit\_params)

Fit to data, then transform it.

Fits transformer to X and y with optional parameters *fit\_params* and returns a transformed version of X.

# Parameters

- X (array-like of shape (n\_samples, n\_features)) Input samples.
- **y** (array-like of shape (n\_samples,) or (n\_samples, n\_outputs), default=None) Target values (None for unsupervised transformations).
- **\*\*fit\_params** (*dict*) Additional fit parameters.

#### Returns

**X\_new** – Transformed array.

#### **Return type**

ndarray array of shape (n\_samples, n\_features\_new)

# get\_feature\_names\_out(input\_features=None)

Mask feature names according to selected features.

#### **Parameters**

input\_features(array-like of str or None, default=None) - Input features.

- If *input\_features* is *None*, then *feature\_names\_in\_* is used as feature names in. If *feature\_names\_in\_* is not defined, then the following input feature names are generated: ["x0", "x1", ..., "x(n\_features\_in\_ 1)"].
- If *input\_features* is an array-like, then *input\_features* must match *feature\_names\_in\_* if *feature\_names\_in\_* is defined.

## Returns

feature\_names\_out – Transformed feature names.

#### **Return type**

ndarray of str objects

### get\_metadata\_routing()

Raise NotImplementedError.

This estimator does not support metadata routing yet.

### get\_params(deep=True)

Get parameters for this estimator.

#### **Parameters**

**deep** (*bool*, *default=True*) – If True, will return the parameters for this estimator and contained subobjects that are estimators.

### Returns

params - Parameter names mapped to their values.

# **Return type**

dict

### get\_support(indices=False)

Get a mask, or integer index, of the features selected.

### Parameters

**indices** (*bool*, *default=False*) – If True, the return value will be an array of integers, rather than a boolean mask.

#### Returns

**support** – An index that selects the retained features from a feature vector. If *indices* is False, this is a boolean array of shape [# input features], in which an element is True iff its corresponding feature is selected for retention. If *indices* is True, this is an integer array of shape [# output features] whose values are indices into the input feature vector.

#### **Return type**

array

# inverse\_transform(X)

Reverse the transformation operation.

# Parameters

**X** (array of shape [n\_samples, n\_selected\_features]) – The input samples.

## Returns

 $X_r - X$  with columns of zeros inserted where features would have been removed by transform().

### **Return type**

array of shape [n\_samples, n\_original\_features]

predict(x\_data, \*\*predict\_kwargs)

Expand predict () to accept kwargs.

### predict\_log\_proba(X)

Predict class log-probabilities for X.

## Parameters

X (array of shape [n\_samples, n\_features]) – The input samples.

#### Returns

 $\mathbf{p}$  – The class log-probabilities of the input samples. The order of the classes corresponds to that in the attribute classes\_.

### **Return type**

array of shape (n\_samples, n\_classes)

## predict\_proba(X)

Predict class probabilities for X.

### **Parameters**

**X** ({array-like or sparse matrix} of shape (n\_samples, n\_features)) – The input samples. Internally, it will be converted to dtype=np.float32 and if a sparse matrix is provided to a sparse csr\_matrix.

#### Returns

 $p-\mbox{The class probabilities of the input samples. The order of the classes corresponds to that in the attribute classes_.$ 

### **Return type**

array of shape (n\_samples, n\_classes)

# score(X, y, \*\*fit\_params)

Reduce X to the selected features and return the score of the estimator.

#### Parameters

- X (array of shape [n\_samples, n\_features]) The input samples.
- y (array of shape [n\_samples]) The target values.
- **\*\*fit\_params** (*dict*) Parameters to pass to the *score* method of the underlying estimator.

Added in version 1.0.

# Returns

**score** – Score of the underlying base estimator computed with the selected features returned by rfe.transform(X) and y.

### **Return type**

float

set\_fit\_request(\*, groups: bool | None | str = 'UNCHANGED', x\_data: bool | None | str = 'UNCHANGED', y\_data: bool | None | str = 'UNCHANGED')  $\rightarrow$  AdvancedRFECV

Request metadata passed to the fit method.

Note that this method is only relevant if enable\_metadata\_routing=True (see sklearn. set\_config()). Please see User Guide on how the routing mechanism works.

The options for each parameter are:

• True: metadata is requested, and passed to fit if provided. The request is ignored if metadata is not provided.

- False: metadata is not requested and the meta-estimator will not pass it to fit.
- None: metadata is not requested, and the meta-estimator will raise an error if the user provides it.
- str: metadata should be passed to the meta-estimator with this given alias instead of the original name.

The default (sklearn.utils.metadata\_routing.UNCHANGED) retains the existing request. This allows you to change the request for some parameters and not others.

Added in version 1.3.

**Note:** This method is only relevant if this estimator is used as a sub-estimator of a meta-estimator, e.g. used inside a Pipeline. Otherwise it has no effect.

### **Parameters**

- groups (str, True, False, or None, default=sklearn.utils. metadata\_routing.UNCHANGED) - Metadata routing for groups parameter in fit.
- **x\_data** (str, True, False, or None, default=sklearn.utils. metadata\_routing.UNCHANGED) - Metadata routing for x\_data parameter in fit.
- y\_data (str, True, False, or None, default=sklearn.utils. metadata\_routing.UNCHANGED) Metadata routing for y\_data parameter in fit.

# Returns

self – The updated object.

## Return type

object

#### set\_output(\*, transform=None)

Set output container.

See Introducing the set\_output API for an example on how to use the API.

### **Parameters**

**transform** ({"default", "pandas"}, default=None) – Configure output of *transform* and *fit\_transform*.

- "default": Default output format of a transformer
- "pandas": DataFrame output
- "polars": Polars output
- None: Transform configuration is unchanged

Added in version 1.4: "polars" option was added.

#### Returns

**self** – Estimator instance.

#### **Return type**

estimator instance

#### set\_params(\*\*params)

Set the parameters of this estimator.

The method works on simple estimators as well as on nested objects (such as Pipeline). The latter have parameters of the form <component>\_\_<parameter> so that it's possible to update each component of a nested object.

## **Parameters**

**\*\*params** (*dict*) – Estimator parameters.

Returns

**self** – Estimator instance.

# **Return type**

estimator instance

 $set\_predict\_request(*, x\_data: bool | None | str = '$UNCHANGED$') \rightarrow AdvancedRFECV$ 

Request metadata passed to the predict method.

Note that this method is only relevant if enable\_metadata\_routing=True (see sklearn. set\_config()). Please see User Guide on how the routing mechanism works.

The options for each parameter are:

- True: metadata is requested, and passed to predict if provided. The request is ignored if metadata is not provided.
- False: metadata is not requested and the meta-estimator will not pass it to predict.
- None: metadata is not requested, and the meta-estimator will raise an error if the user provides it.
- str: metadata should be passed to the meta-estimator with this given alias instead of the original name.

The default (sklearn.utils.metadata\_routing.UNCHANGED) retains the existing request. This allows you to change the request for some parameters and not others.

Added in version 1.3.

**Note:** This method is only relevant if this estimator is used as a sub-estimator of a meta-estimator, e.g. used inside a Pipeline. Otherwise it has no effect.

# Parameters

x\_data (str, True, False, or None, default=sklearn.utils. metadata\_routing.UNCHANGED) - Metadata routing for x\_data parameter in predict.

Returns

self – The updated object.

**Return type** 

object

#### transform(X)

Reduce X to the selected features.

# Parameters

**X** (array of shape [n\_samples, n\_features]) – The input samples.

### Returns

 $X_r$  – The input samples with only the selected features.

## **Return type**

array of shape [n\_samples, n\_selected\_features]

class esmvaltool.diag\_scripts.mlr.custom\_sklearn.AdvancedTransformedTargetRegressor(regressor=None,

\*, transformer=None, func=None, inverse\_func=None, check\_inverse=True)

Bases: TransformedTargetRegressor

Expand sklearn.compose.TransformedTargetRegressor.

# property coef\_

Model coefficients.

Туре

numpy.ndarray

# property feature\_importances\_

Feature importances.

Туре

numpy.ndarray

fit(x\_data, y\_data, \*\*fit\_kwargs)

Expand fit() to accept kwargs.

### fit\_transformer\_only(y\_data, \*\*fit\_kwargs)

Fit only transformer step.

# get\_metadata\_routing()

Raise NotImplementedError.

This estimator does not support metadata routing yet.

# get\_params(deep=True)

Get parameters for this estimator.

# Parameters

**deep** (*bool*, *default=True*) – If True, will return the parameters for this estimator and contained subobjects that are estimators.

### Returns

params – Parameter names mapped to their values.

# **Return type**

dict

# property n\_features\_in\_

Number of features seen during fit.

# predict(x\_data, always\_return\_1d=True, \*\*predict\_kwargs)

Expand predict () to accept kwargs.

### score(X, y, sample\_weight=None)

Return the coefficient of determination of the prediction.

The coefficient of determination  $R^2$  is defined as  $(1-\frac{u}{v})$ , where u is the residual sum of squares ((y\_true - y\_pred)\*\* 2).sum() and v is the total sum of squares ((y\_true - y\_true.mean()) \*\* 2). sum(). The best possible score is 1.0 and it can be negative (because the model can be arbitrarily worse). A constant model that always predicts the expected value of y, disregarding the input features, would get a  $R^2$  score of 0.0.

### Parameters

- X (array-like of shape (n\_samples, n\_features)) Test samples. For some estimators this may be a precomputed kernel matrix or a list of generic objects instead with shape (n\_samples, n\_samples\_fitted), where n\_samples\_fitted is the number of samples used in the fitting for the estimator.
- **y** (array-like of shape (n\_samples,) or (n\_samples, n\_outputs)) True values for *X*.
- **sample\_weight** (array-like of shape (n\_samples,), default=None) Sample weights.

## Returns

**score**  $-R^2$  of self.predict(X) w.r.t. y.

# Return type

float

## Notes

The  $R^2$  score used when calling score on a regressor uses multioutput='uniform\_average' from version 0.23 to keep consistent with default value of r2\_score(). This influences the score method of all the multioutput regressors (except for MultiOutputRegressor).

```
set_fit_request(*, x_data: bool | None | str = '$UNCHANGED$', y_data: bool | None | str = '$UNCHANGED$') \rightarrow AdvancedTransformedTargetRegressor
```

Request metadata passed to the fit method.

Note that this method is only relevant if enable\_metadata\_routing=True (see sklearn. set\_config()). Please see User Guide on how the routing mechanism works.

The options for each parameter are:

- True: metadata is requested, and passed to fit if provided. The request is ignored if metadata is not provided.
- False: metadata is not requested and the meta-estimator will not pass it to fit.
- None: metadata is not requested, and the meta-estimator will raise an error if the user provides it.
- str: metadata should be passed to the meta-estimator with this given alias instead of the original name.

The default (sklearn.utils.metadata\_routing.UNCHANGED) retains the existing request. This allows you to change the request for some parameters and not others.

Added in version 1.3.

**Note:** This method is only relevant if this estimator is used as a sub-estimator of a meta-estimator, e.g. used inside a Pipeline. Otherwise it has no effect.

# Parameters

- **x\_data** (str, True, False, or None, default=sklearn.utils. metadata\_routing.UNCHANGED) - Metadata routing for x\_data parameter in fit.
- y\_data (str, True, False, or None, default=sklearn.utils. metadata\_routing.UNCHANGED) Metadata routing for y\_data parameter in fit.

#### Returns

self – The updated object.

**Return type** 

object

#### set\_params(\*\*params)

Set the parameters of this estimator.

The method works on simple estimators as well as on nested objects (such as Pipeline). The latter have parameters of the form <component>\_\_<parameter> so that it's possible to update each component of a nested object.

```
Parameters
**params (dict) – Estimator parameters.
```

**Returns self** – Estimator instance.

### **Return type**

estimator instance

```
set\_predict\_request(*, always\_return\_1d: bool | None | str = '$UNCHANGED$', x\_data: bool | None | str = '$UNCHANGED$') \rightarrow AdvancedTransformedTargetRegressor
```

Request metadata passed to the predict method.

Note that this method is only relevant if enable\_metadata\_routing=True (see sklearn. set\_config()). Please see User Guide on how the routing mechanism works.

The options for each parameter are:

- True: metadata is requested, and passed to predict if provided. The request is ignored if metadata is not provided.
- False: metadata is not requested and the meta-estimator will not pass it to predict.
- None: metadata is not requested, and the meta-estimator will raise an error if the user provides it.
- str: metadata should be passed to the meta-estimator with this given alias instead of the original name.

The default (sklearn.utils.metadata\_routing.UNCHANGED) retains the existing request. This allows you to change the request for some parameters and not others.

Added in version 1.3.

**Note:** This method is only relevant if this estimator is used as a sub-estimator of a meta-estimator, e.g. used inside a Pipeline. Otherwise it has no effect.

# Parameters

- always\_return\_1d (str, True, False, or None, default=sklearn. utils.metadata\_routing.UNCHANGED) - Metadata routing for always\_return\_1d parameter in predict.
- **x\_data** (str, True, False, or None, default=sklearn.utils. metadata\_routing.UNCHANGED) - Metadata routing for x\_data parameter in predict.

### Returns

self – The updated object.

**Return type** 

object

set\_score\_request(\*, sample\_weight: bool | None |  $str = '$UNCHANGED$') \rightarrow AdvancedTransformedTargetRegressor$ 

Request metadata passed to the score method.

Note that this method is only relevant if enable\_metadata\_routing=True (see sklearn. set\_config()). Please see User Guide on how the routing mechanism works.

The options for each parameter are:

- True: metadata is requested, and passed to score if provided. The request is ignored if metadata is not provided.
- False: metadata is not requested and the meta-estimator will not pass it to score.
- None: metadata is not requested, and the meta-estimator will raise an error if the user provides it.
- str: metadata should be passed to the meta-estimator with this given alias instead of the original name.

The default (sklearn.utils.metadata\_routing.UNCHANGED) retains the existing request. This allows you to change the request for some parameters and not others.

Added in version 1.3.

**Note:** This method is only relevant if this estimator is used as a sub-estimator of a meta-estimator, e.g. used inside a Pipeline. Otherwise it has no effect.

### Parameters

sample\_weight (str, True, False, or None, default=sklearn.utils. metadata\_routing.UNCHANGED) - Metadata routing for sample\_weight parameter in score.

#### Returns

self – The updated object.

# **Return type**

object

# 

ranking, support)

# Bases: BaseEstimator, SelectorMixin

Transformer step of a feature selection estimator.

**fit**(\*\_, \*\*\_\_)

Empty method.

## fit\_transform(X, y=None, \*\*fit\_params)

Fit to data, then transform it.

Fits transformer to X and y with optional parameters *fit\_params* and returns a transformed version of X.

#### **Parameters**

- X (array-like of shape (n\_samples, n\_features)) Input samples.
- **y** (array-like of shape (n\_samples,) or (n\_samples, n\_outputs), default=None) Target values (None for unsupervised transformations).
- **\*\*fit\_params** (*dict*) Additional fit parameters.

### Returns

**X\_new** – Transformed array.

### **Return type**

ndarray array of shape (n\_samples, n\_features\_new)

### get\_feature\_names\_out(input\_features=None)

Mask feature names according to selected features.

## Parameters

**input\_features** (array-like of str or None, default=None) – Input features.

- If *input\_features* is *None*, then *feature\_names\_in\_* is used as feature names in. If *feature\_names\_in\_* is not defined, then the following input feature names are generated: ["x0", "x1", ..., "x(n\_features\_in\_ 1)"].
- If *input\_features* is an array-like, then *input\_features* must match *feature\_names\_in\_* if *feature\_names\_in\_* is defined.

# Returns

feature\_names\_out – Transformed feature names.

#### **Return type**

ndarray of str objects

# get\_metadata\_routing()

Get metadata routing of this object.

Please check User Guide on how the routing mechanism works.

# Returns

routing - A MetadataRequest encapsulating routing information.

### **Return type**

MetadataRequest

#### get\_params(deep=True)

Get parameters for this estimator.

### **Parameters**

**deep** (*bool*, *default=True*) – If True, will return the parameters for this estimator and contained subobjects that are estimators.

# Returns

params - Parameter names mapped to their values.

# **Return type**

dict

# get\_support(indices=False)

Get a mask, or integer index, of the features selected.

# Parameters

**indices** (*bool*, *default=False*) – If True, the return value will be an array of integers, rather than a boolean mask.

#### Returns

**support** – An index that selects the retained features from a feature vector. If *indices* is False, this is a boolean array of shape [# input features], in which an element is True iff its corresponding feature is selected for retention. If *indices* is True, this is an integer array of shape [# output features] whose values are indices into the input feature vector.

### **Return type**

array

### inverse\_transform(X)

Reverse the transformation operation.

#### Parameters

X (array of shape [n\_samples, n\_selected\_features]) – The input samples.

### Returns

 $X_r - X$  with columns of zeros inserted where features would have been removed by transform().

## **Return type**

array of shape [n\_samples, n\_original\_features]

### set\_output(\*, transform=None)

Set output container.

See Introducing the set\_output API for an example on how to use the API.

#### Parameters

**transform** ({"default", "pandas"}, default=None) – Configure output of *transform* and *fit\_transform*.

- "default": Default output format of a transformer
- "pandas": DataFrame output
- "polars": Polars output
- None: Transform configuration is unchanged

Added in version 1.4: "polars" option was added.

#### Returns

self – Estimator instance.

#### **Return type**

estimator instance

# set\_params(\*\*params)

Set the parameters of this estimator.

The method works on simple estimators as well as on nested objects (such as Pipeline). The latter have parameters of the form <component>\_\_<parameter> so that it's possible to update each component of a nested object.

**Parameters** \*\*params (*dict*) – Estimator parameters.

Returns

**self** – Estimator instance.

Return type estimator instance

## transform(X)

Reduce X to the selected features.

## Parameters

X (array of shape [n\_samples, n\_features]) – The input samples.

### Returns

 $X_r$  – The input samples with only the selected features.

### **Return type**

array of shape [n\_samples, n\_selected\_features]

esmvaltool.diag\_scripts.mlr.custom\_sklearn.cross\_val\_score\_weighted(estimator, x\_data,

y\_data=None, groups=None, scoring=None, cv=None, n\_jobs=None, verbose=0, fit\_params=None, pre\_dispatch='2\*n\_jobs', error\_score=nan, sample\_weights=None)

### Expand sklearn.model\_selection.cross\_val\_score().

esmvaltool.diag\_scripts.mlr.custom\_sklearn.get\_rfecv\_transformer(rfecv\_estimator)
Get transformer step of RFECV estimator.

esmvaltool.diag\_scripts.mlr.custom\_sklearn.perform\_efecv(estimator, x\_data, y\_data, \*\*kwargs)
Perform exhaustive feature selection.

# **MLRModel base class**

Base class for MLR models.

# **Example recipe**

The *MLR main diagnostic script* provides an interface for using MLR models in recipes. The following recipe shows a typical example on how to setup MLR recipes/diagnostics with the following properties:

- Setup an MLR model with target variable y (using the tag Y) and three predictors x1, x2 and latitude (with tags X1, X2 and latitude, respectively). The target variable needs the attribute var\_type: label; the predictors x1 and x2 the attribute var\_type: feature. The coordinate feature latitude is added via the option coords\_as\_features: [latitude].
- 2. Suppose y and x1 are 3D fields (pressure, latitude, longitude); x2 is a 2D field (latitude, longitude). Thus, it is necessary to add the attribute broadcast\_from: [1, 2] to it (see dim\_map parameter in iris.util. broadcast\_to\_shape() for details). In order to consider multiple climate models (A, B and C) at once, the option group\_datasets\_by\_attributes: [dataset] is necessary. Otherwise the diagnostic will complain about duplicate data.
- 3. For the prediction, data from dataset D is used (with var\_type: prediction\_input). For the feature X1 additional input error (with var\_type: prediction\_input\_error) is used.

```
diag feature x1:
 variables:
    feature:
      ... # specify project, mip, start_year, end_year, etc.
      short_name: x1
      var_type: feature
      tag: X1
      additional_datasets:
        - {dataset: A, ...}
        - {dataset: B, ...}
        - {dataset: C, ...}
    prediction_input:
      ... # specify project, mip, start_year, end_year, etc.
      short_name: x1
      var_type: prediction_input
      tag: X1
      additional_datasets:
        - {dataset: D, ...}
    prediction_input_error:
      ... # specify project, mip, start_year, end_year, etc.
      short_name: x1Stderr
      var_type: prediction_input_error
      tag: X1
      additional_datasets:
        - {dataset: D, ...}
  scripts:
    null
diag_feature_x2:
  variables:
    feature:
      ... # specify project, mip, start_year, end_year, etc.
      short_name: x2
      var_type: feature
      broadcast_from: [1, 2]
      tag: X2
```

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```
additional_datasets:
        - {dataset: A, ...}
        - {dataset: B, ...}
        - {dataset: C, ...}
    prediction_input:
      ... # specify project, mip, start_year, end_year, etc.
      short_name: x2
      var_type: prediction_input
      broadcast_from: [1, 2]
      tag: X2
      additional_datasets:
        - {dataset: D, ...}
  scripts:
    null
diag_label:
 variables:
    label:
      ... # specify project, mip, start_year, end_year, etc.
      short_name: y
      var_type: label
      tag: Y
      additional_datasets:
        - {dataset: A, ...}
        - {dataset: B, ...}
        - {dataset: C, ...}
  scripts:
    null
```

- 4. In this example, a GBRT model (with mlr\_model\_type: gbr\_sklearn) is used. Parameters for this are specified via parameters\_final\_regressor. Apart from the best-estimate prediction, the estimated MLR model error (save\_mlr\_model\_error: test) and the propagated prediction input error (save\_propagated\_errors: true) are returned.
- 5. With postprocess.py, the global mean of the best estimate prediction and the corresponding errors (MLR model + propagated input error) are calculted.

```
diag_mlr_gbrt:
  scripts:
   mlr:
      script: mlr/main.py
      ancestors: [
         'diag_label/y'.
         'diag_feature_*/*',
      1
      coords_as_features: [latitude]
      group_datasets_by_attributes: [dataset]
      mlr_model_name: GBRT
     mlr_model_type: gbr_sklearn
      parameters_final_regressor:
        learning_rate: 0.1
        n_estimators: 100
      save_mlr_model_error: test
```

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```
save_propagated_errors: true
postprocess:
    script: mlr/postprocess.py
    ancestors: ['diag_mlr_gbrt/mlr']
    ignore:
        - {var_type: null}
    mean: [pressure, latitude, longitude]
```

6. Plots of the global distribution (latitude, longitude) are created with plot.py after calculating the mean over the pressure coordinate using preprocess.py.

```
diag_plot:
  scripts:
   preprocess:
      script: mlr/preprocess.py
      ancestors: ['diag_mlr_gbrt/mlr']
      collapse: [pressure]
      ignore:
        - {var_type: null}
   plot:
      script: mlr/plot.py
      ancestors: ['diag_plot/preprocess']
     plot_map:
         plot_kwargs:
           cbar_label: 'Y'
           cbar_ticks: [0, 1, 2, 3]
           vmin: 0
           vmax: 3
```

All datasets must have the attribute var\_type which specifies the type of the dataset. Possible values are feature (independent variables used for training/testing), label (dependent variables, y-axis), prediction\_input (independent variables used for prediction of dependent variables, usually observational data), prediction\_input\_error (standard error of the prediction\_input data, optional) or prediction\_reference (*true* values for the prediction\_linput data, optional). In addition, all datasets must habe the attribute tag, which specifies the name of variable/diagnostic. All datasets can be converted to new units in the loading step by specifying the key convert\_units\_to in the respective dataset(s).

# **Training data**

All groups (specified in group\_datasets\_by\_attributes, if desired) given for label datasets must also be given for the feature datasets. Within these groups, all feature and label datasets must have the same shape, except the attribute broadcast\_from is set to a list of suitable coordinate indices to map this dataset to regular datasets (see parameter dim\_map in iris.util.broadcast\_to\_shape()).

# **Prediction data**

All tag s specified for prediction\_input datasets must also be given for the feature datasets (except allow\_missing\_features is set to True). Multiple predictions can be specified by prediction\_name. Within these predictions, all prediction\_input datasets must have the same shape, except the attribute broadcast\_from is given. Errors in the prediction input data can be specified by prediction\_input\_error. If given, these errors are used to calculate errors in the final prediction using linear error propagation given by LIME. Additionally, *true* values for prediction\_input can be specified with prediction\_reference datasets (together with the respective prediction\_name). This allows an evaluation of the performance of the MLR model by calculating residuals (*true* minus predicted values).

# Available MLR models

MLR models are subclasses of this base class. A list of all available MLR models can be found *here*. To add a new MLR model, create a new file in esmvaltool/diag\_scripts/mlr/models/ with a child class of esmvaltool. diag\_scripts.mlr.models.MLRModel decorated with esmvaltool.diag\_scripts.mlr.models.MLRModel. register\_mlr\_model().

# Optional parameters for class initialization

### accept\_only\_scalar\_data: bool (default: False)

If set to True, only accept scalar input data. Should be used together with the option group\_datasets\_by\_attributes.

### allow\_missing\_features: bool (default: False)

Allow missing features in the training data.

# cache\_intermediate\_results: bool (default: True)

Cache the intermediate results of the pipeline's transformers.

## categorical\_features: list of str

Names of features which are interpreted as categorical features (in contrast to numerical features).

# coords\_as\_features: list of str

If given, specify a list of coordinates which should be used as features.

# dtype: str (default: 'float64')

Internal data type which is used for all calculations, see https://docs.scipy.org/doc/numpy/user/basics.types.html for a list of allowed values.

# fit\_kwargs: dict

Optional keyword arguments for the pipeline's fit() function. These arguments have to be given for each step of the pipeline separated by two underscores, i.e.  $s_p$  is the parameter p for step s.

#### group\_datasets\_by\_attributes: list of str

List of dataset attributes which are used to group input data for feature s and label s. For example, this is necessary if the MLR model should consider multiple climate models in the training phase. If this option is not given, specifying multiple datasets with identical var\_type and tag entries results in an error. If given, all the input data is first grouped by the given attributes and then checked for uniqueness within this group. After that, all groups are stacked to form a single set of training data.

# imputation\_strategy: str (default: 'remove')

Strategy for the imputation of missing values in the features. Must be one of 'remove', 'mean', 'median', 'most\_frequent' or 'constant'.

#### log\_level: str (default: 'info')

Verbosity for the logger. Must be one of 'debug', 'info', 'warning' or 'error'.

# mlr\_model\_name: str

Human-readable name of the MLR model instance (e.g used for labels).

#### n\_jobs: int (default: 1)

Maximum number of jobs spawned by this class. Use -1 to use all processors. More details are given here.

#### output\_file\_type: str (default: 'png')

File type for the plots.

# parameters: dict

Parameters used for the whole pipeline. Have to be given for each step of the pipeline separated by two underscores, i.e. s\_\_p is the parameter p for step s. random\_state parameters are explicitly allowed here (in contrast to parameters\_final\_regressor).

## parameters\_final\_regressor: dict

Parameters used for the **final** regressor. If these parameters are updated using the function update\_parameters(), the new names have to be given for each step of the pipeline separated by two underscores, i.e. s\_\_p is the parameter p for step s. Note: to pass an argument for random\_state, use the option random\_state of this class.

# pca: bool (default: False)

Preprocess numerical input features using PCA. Parameters for this pipeline step can be given via the parameters argument.

# plot\_dir: str (default: ~/plots)

Root directory to save plots.

# plot\_units: dict

Replace specific units (keys) with other text (values) in plots.

#### random\_state: int or None (default: None)

Random seed for numpy.random.RandomState that is used by all functionalities of this class that require randomness (e.g., probabilistic ML algorithms like Gradient Boosting Regression models, random train test splits, etc.). If None, use a random seed. Use an int to get reproducible results. See https://scikit-learn.org/stable/ common\_pitfalls.html#controlling-randomness for more details.

### savefig\_kwargs: dict

Keyword arguments for matplotlib.pyplot.savefig().

#### seaborn\_settings: dict

Options for seaborn.set\_theme() (affects all plots).

### standardize\_data: bool (default: True)

Linearly standardize numerical input data by removing mean and scaling to unit variance.

#### sub\_dir: str

Create additional subdirectory for output in work\_dir and plot\_dir.

# test\_size: float (default: 0.25)

If given, randomly exclude the desired fraction of input data from training and use it as test data.

# weighted\_samples: dict

If specified, use weighted samples in the loss function used for the training of the MLR model. The given keyword arguments are directly passed to *esmvaltool.diag\_scripts.mlr.get\_all\_weights()* to calculate the sample weights. By default, no weights are used. Raises errors if the desired weights cannot be calculated for the data, e.g., when time\_weighted=True is used but the data does not contain a dimension time.

### work\_dir: str (default: ~/work)

Root directory to save all other files (mainly \*.nc files).

# **Classes:**

MLRModel(input\_datasets, \*\*kwargs)

Base class for MLR models.

class esmvaltool.diag\_scripts.mlr.models.MLRModel(input\_datasets, \*\*kwargs)

Bases: object

Base class for MLR models.

# Attributes:

categorical_features	Categorical features.
5	6
data	Input data of the MLR model.
features	Features of the input data.
features_after_preprocessing	Features of the input data after preprocessing.
features_types	Types of the features.
features_units	Units of the features.
fit_kwargs	Keyword arguments for fit().
group_attributes	Group attributes of the input data.
label	Label of the input data.
label_units	Units of the label.
mlr_model_type	MLR model type.
numerical_features	Numerical features.
parameters	Parameters of the complete MLR model pipeline.
random_state	Random state instance.

# Methods:

<pre>create(mlr_model_type, *args, **kwargs)</pre>	Create desired MLR model subclass (factory method).
efecv(**kwargs)	Perform exhaustive feature elimination using cross-validation.
<pre>export_prediction_data([filename])</pre>	Export all prediction data contained in <i>selfdata</i> .
<pre>export_training_data([filename])</pre>	Export all training data contained in selfdata.
fit()	Fit MLR model.
<pre>get_ancestors([label, features,])</pre>	Return ancestor files.
<pre>get_data_frame(data_type[, impute_nans])</pre>	Return data frame of specified type.
<pre>get_x_array(data_type[, impute_nans])</pre>	Return x data of specific type.
<pre>get_y_array(data_type[, impute_nans])</pre>	Return y data of specific type.
<pre>grid_search_cv(param_grid, **kwargs)</pre>	Perform exhaustive parameter search using cross-validation.
<pre>plot_1d_model([filename, n_points])</pre>	Plot lineplot that represents the MLR model.
<pre>plot_partial_dependences([filename])</pre>	Plot partial dependences for every feature.
<pre>plot_prediction_errors([filename])</pre>	Plot predicted vs.
<pre>plot_residuals([filename])</pre>	Plot residuals of training and test (if available) data.
<pre>plot_residuals_distribution([filename])</pre>	Plot distribution of residuals of training and test data (KDE).
<pre>plot_residuals_histogram([filename])</pre>	Plot histogram of residuals of training and test data.
<pre>plot_scatterplots([filename])</pre>	Plot scatterplots label vs.
<pre>predict([save_mlr_model_error,])</pre>	Perform prediction using the MLR model(s) and write *.nc files.
<pre>print_correlation_matrices()</pre>	Print correlation matrices for all datasets.
<pre>print_regression_metrics([logo])</pre>	Print all available regression metrics for training data.
<pre>register_mlr_model(mlr_model_type)</pre>	Add MLR model (subclass of this class) (decorator).
reset_pipeline()	Reset regressor pipeline.
<pre>rfecv(**kwargs)</pre>	Perform recursive feature elimination using cross-validation.
<pre>test_normality_of_residuals()</pre>	Perform Shapiro-Wilk test to normality of residuals.
<pre>update_parameters(**params)</pre>	Update parameters of the whole pipeline.

# property categorical\_features

Categorical features.

Туре

numpy.ndarray

classmethod create(mlr\_model\_type, \*args, \*\*kwargs)

Create desired MLR model subclass (factory method).

# property data

Input data of the MLR model.

Type dict

# efecv(\*\*kwargs)

Perform exhaustive feature elimination using cross-validation.

```
**kwargs (keyword arguments, optional) – Additional options for esmvaltool. diag_scripts.mlr. custom_sklearn.cross_val_score_weighted().
```

## export\_prediction\_data(filename=None)

Export all prediction data contained in *self.\_data*.

# Parameters

**filename** (*str*, *optional* (*default: '{data\_type}\_{pred\_name}.csv'*)) – Name of the exported files.

# export\_training\_data(filename=None)

Export all training data contained in *self.\_data*.

#### **Parameters**

**filename** (*str*, *optional* (*default:* '{*data\_type*}.*csv*')) - Name of the exported files.

### property features

Features of the input data.

Туре

numpy.ndarray

## property features\_after\_preprocessing

Features of the input data after preprocessing.

Туре

numpy.ndarray

# property features\_types

Types of the features.

Type

pandas.Series

## property features\_units

Units of the features.

Туре

pandas.Series

# fit()

Fit MLR model.

**Note:** Specifying keyword arguments for this function is not allowed here since *features\_after\_preprocessing* might be altered by that. Use the keyword argument fit\_kwargs during class initialization instead.

# property fit\_kwargs

Keyword arguments for fit().

Type dict

get\_ancestors(label=True, features=None, prediction\_names=None, prediction\_reference=False)

Return ancestor files.

- label (bool, optional (default: True)) Return label files.
- **features** (*list of str*, *optional* (*default: None*)) Features for which files should be returned. If None, return files for all features.

- **prediction\_names** (list of str, optional (default: None)) Prediction names for which files should be returned. If None, return files for all prediction names.
- prediction\_reference (bool, optional (default: False)) Return prediction\_reference files if available for given prediction\_names.

# Returns

Ancestor files.

# **Return type**

list of str

## Raises

**ValueError** – Invalid feature or prediction\_name given.

#### get\_data\_frame(data\_type, impute\_nans=False)

Return data frame of specified type.

### **Parameters**

- **data\_type** (*str*) Data type to be returned. Must be one of 'all', 'train' or 'test'.
- impute\_nans (bool, optional (default: False)) Impute nans if desired.

#### Returns

Desired data.

# **Return type**

pandas.DataFrame

### Raises

**TypeError** – data\_type is invalid or data does not exist (e.g. test data is not set).

### get\_x\_array(data\_type, impute\_nans=False)

Return x data of specific type.

# Parameters

- **data\_type** (*str*) Data type to be returned. Must be one of 'all', 'train' or 'test'.
- impute\_nans (bool, optional (default: False)) Impute nans if desired.

# Returns

Desired data.

# Return type

numpy.ndarray

### Raises

**TypeError** – data\_type is invalid or data does not exist (e.g. test data is not set).

# get\_y\_array(data\_type, impute\_nans=False)

Return y data of specific type.

- **data\_type** (*str*) Data type to be returned. Must be one of 'all', 'train' or 'test'.
- impute\_nans (bool, optional (default: False)) Impute nans if desired.

# Returns

Desired data.

# **Return type**

numpy.ndarray

# Raises

**TypeError** – data\_type is invalid or data does not exist (e.g. test data is not set).

### grid\_search\_cv(param\_grid, \*\*kwargs)

Perform exhaustive parameter search using cross-validation.

### **Parameters**

- **param\_grid** (*dict or list of dict*) Parameter names (keys) and ranges (values) for the search. Have to be given for each step of the pipeline separated by two underscores, i.e. s\_\_p is the parameter p for step s.
- **\*\*kwargs** (*keyword arguments, optional*) Additional options for sklearn. model\_selection.GridSearchCV.

# Raises

**ValueError** – Final regressor does not supply the attributes best\_estimator\_ or best\_params\_.

# property group\_attributes

Group attributes of the input data.

Туре

numpy.ndarray

# property label

Label of the input data.

Type str

property label\_units

Units of the label.

Type str

511

property mlr\_model\_type

MLR model type.

# Туре

str

# property numerical\_features

Numerical features.

# Туре

numpy.ndarray

## property parameters

Parameters of the complete MLR model pipeline.

Туре

dict

#### plot\_1d\_model(filename=None, n\_points=1000)

Plot lineplot that represents the MLR model.

**Note:** This only works for a model with a single feature.

# Parameters

- **filename** (*str*, *optional* (*default: '1d\_mlr\_model'*)) Name of the plot file.
- **n\_points** (*int*, *optional* (*default:* 1000)) Number of sampled points for the single feature (using linear spacing between minimum and maximum value).

### Raises

- sklearn.exceptions.NotFittedError MLR model is not fitted.
- ValueError MLR model is built from more than 1 feature.

## plot\_partial\_dependences(filename=None)

Plot partial dependences for every feature.

# Parameters

filename (str, optional (default: 'partial\_dependece\_{feature}')) Name of the plot file.

#### Raises

sklearn.exceptions.NotFittedError - MLR model is not fitted.

# plot\_prediction\_errors(filename=None)

Plot predicted vs. true values.

# Parameters

**filename** (*str*, *optional* (*default: 'prediction\_errors'*)) – Name of the plot file.

### Raises

sklearn.exceptions.NotFittedError – MLR model is not fitted.

#### plot\_residuals(filename=None)

Plot residuals of training and test (if available) data.

# Parameters

**filename** (*str*, *optional* (*default:* '*residuals*')) – Name of the plot file.

#### Raises

sklearn.exceptions.NotFittedError – MLR model is not fitted.

# plot\_residuals\_distribution(filename=None)

Plot distribution of residuals of training and test data (KDE).

### **Parameters**

**filename** (*str*, *optional* (*default: 'residuals\_distribution'*)) – Name of the plot file.

#### Raises

sklearn.exceptions.NotFittedError – MLR model is not fitted.

#### plot\_residuals\_histogram(filename=None)

Plot histogram of residuals of training and test data.

### Parameters

**filename** (*str*, *optional* (*default: 'residuals\_histogram'*)) – Name of the plot file.

#### Raises

sklearn.exceptions.NotFittedError – MLR model is not fitted.

### plot\_scatterplots(filename=None)

Plot scatterplots label vs. feature for every feature.

### Parameters

**filename** (*str*, *optional* (*default:* '*scatterplot\_{feature}*')) – Name of the plot file.

### Raises

#### sklearn.exceptions.NotFittedError – MLR model is not fitted.

Perform prediction using the MLR model(s) and write \*.nc files.

#### **Parameters**

- save\_mlr\_model\_error (str or int, optional) Additionally saves estimated squared MLR model error. This error represents the uncertainty of the prediction caused by the MLR model itself and not by errors in the prediction input data (errors in that will be considered by including datasets with var\_type set to prediction\_input\_error and setting save\_propagated\_errors to True). If the option is set to 'test', the (constant) error is estimated as RMSEP using a (hold-out) test data set. Only possible if test data is available, i.e. the option test\_size is not set to False during class initialization. If the option is set to 'logo', the (constant) error is estimated as RMSEP using the group\_attributes. Only possible if group\_datasets\_by\_attributes is given. If the option is set to an integer n (!= 0), the (constant) error is estimated as RMSEP using n-fold cross-validation.
- **save\_lime\_importance** (*bool*, *optional* (*default: False*)) Additionally saves local feature importance given by LIME (Local Interpretable Model-agnostic Explanations).
- **save\_propagated\_errors** (*bool*, *optional* (*default: False*)) Additionally saves propagated errors from prediction\_input\_error datasets. Only possible when these are available.
- **\*\*kwargs** (*keyword arguments*, *optional*) Additional options for the final regressors predict() function.

#### Raises

- **RuntimeError** return\_var and return\_cov are both set to True.
- sklearn.exceptions.NotFittedError MLR model is not fitted.
- ValueError An invalid value for save\_mlr\_model\_error is given.
- **ValueError** save\_propagated\_errors is True and no prediction\_input\_error data is available.

#### print\_correlation\_matrices()

Print correlation matrices for all datasets.

#### print\_regression\_metrics(logo=False)

Print all available regression metrics for training data.

### Parameters

**logo** (bool, optional (default: False)) – Print regression metrics using sklearn.model\_selection.LeaveOneGroupOut cross-validation. Only possible when group\_datasets\_by\_attributes was given during class initialization.

# property random\_state

Random state instance.

Туре

numpy.random.RandomState

### classmethod register\_mlr\_model(mlr\_model\_type)

Add MLR model (subclass of this class) (decorator).

## reset\_pipeline()

Reset regressor pipeline.

# rfecv(\*\*kwargs)

Perform recursive feature elimination using cross-validation.

**Note:** This only works for final estimators that provide information about feature importance either through a coef\_ attribute or through a feature\_importances\_ attribute.

#### **Parameters**

```
**kwargs (keyword arguments, optional) - Additional options for sklearn. feature_selection.RFECV.
```

## Raises

**RuntimeError** – Final estimator does not provide coef\_ or feature\_importances\_ attribute.

# test\_normality\_of\_residuals()

Perform Shapiro-Wilk test to normality of residuals.

#### Raises

sklearn.exceptions.NotFittedError – MLR model is not fitted.

### update\_parameters(\*\*params)

Update parameters of the whole pipeline.

**Note:** Parameter names have to be given for each step of the pipeline separated by two underscores, i.e. s\_\_p is the parameter p for step s.

# Parameters

**\*\*params** (keyword arguments, optional) – Parameters for the pipeline which should be updated.

### Raises

**ValueError** – Invalid parameter for pipeline given.

# **Base class for Gradient Boosted Regression models**

Base class for Gradient Boosting Regression model.

**Classes:** 

GBRMode1(input_datasets, **kwargs) Ba	Base class for Gradient Boosting Regression models.
---------------------------------------	---

class esmvaltool.diag\_scripts.mlr.models.gbr\_base.GBRModel(input\_datasets, \*\*kwargs)

Bases: MLRModel

Base class for Gradient Boosting Regression models.

# Attributes:

categorical_features	Categorical features.
data	Input data of the MLR model.
features	Features of the input data.
features_after_preprocessing	Features of the input data after preprocessing.
features_types	Types of the features.
features_units	Units of the features.
fit_kwargs	Keyword arguments for fit().
group_attributes	Group attributes of the input data.
label	Label of the input data.
label_units	Units of the label.
mlr_model_type	MLR model type.
numerical_features	Numerical features.
parameters	Parameters of the complete MLR model pipeline.
random_state	Random state instance.

# Methods:

<pre>create(mlr_model_type, *args, **kwargs)</pre>	Create desired MLR model subclass (factory method).
efecv(**kwargs)	Perform exhaustive feature elimination using cross-validation.
<pre>export_prediction_data([filename])</pre>	Export all prediction data contained in <i>selfdata</i> .
<pre>export_training_data([filename])</pre>	Export all training data contained in <i>selfdata</i> .
fit()	Fit MLR model.
<pre>get_ancestors([label, features,])</pre>	Return ancestor files.
<pre>get_data_frame(data_type[, impute_nans])</pre>	Return data frame of specified type.
<pre>get_x_array(data_type[, impute_nans])</pre>	Return x data of specific type.
<pre>get_y_array(data_type[, impute_nans])</pre>	Return y data of specific type.
<i>grid_search_cv</i> (param_grid, **kwargs)	Perform exhaustive parameter search using cross-validation.
<pre>plot_1d_model([filename, n_points])</pre>	Plot lineplot that represents the MLR model.
<pre>plot_feature_importance([filename,</pre>	Plot feature importance.
color_coded])	
<pre>plot_partial_dependences([filename])</pre>	Plot partial dependences for every feature.
<pre>plot_prediction_errors([filename])</pre>	Plot predicted vs.
<pre>plot_residuals([filename])</pre>	Plot residuals of training and test (if available) data.
<pre>plot_residuals_distribution([filename])</pre>	Plot distribution of residuals of training and test data (KDE).
<pre>plot_residuals_histogram([filename])</pre>	Plot histogram of residuals of training and test data.
<pre>plot_scatterplots([filename])</pre>	Plot scatterplots label vs.
<pre>predict([save_mlr_model_error,])</pre>	Perform prediction using the MLR model(s) and write *.nc files.
<pre>print_correlation_matrices()</pre>	Print correlation matrices for all datasets.
<pre>print_regression_metrics([logo])</pre>	Print all available regression metrics for training data.
<pre>register_mlr_model(mlr_model_type)</pre>	Add MLR model (subclass of this class) (decorator).
reset_pipeline()	Reset regressor pipeline.
<pre>rfecv(**kwargs)</pre>	Perform recursive feature elimination using cross-validation.
<pre>test_normality_of_residuals()</pre>	Perform Shapiro-Wilk test to normality of residuals.
<pre>update_parameters(**params)</pre>	Update parameters of the whole pipeline.

# property categorical\_features

Categorical features.

## Туре

numpy.ndarray

classmethod create(mlr\_model\_type, \*args, \*\*kwargs)
Create desired MLR model subclass (factory method).

# property data

Input data of the MLR model.

Туре

dict

# efecv(\*\*kwargs)

Perform exhaustive feature elimination using cross-validation.

```
**kwargs (keyword arguments, optional) – Additional options for esmvaltool. diag_scripts.mlr. custom_sklearn.cross_val_score_weighted().
```

## export\_prediction\_data(filename=None)

Export all prediction data contained in *self.\_data*.

# Parameters

**filename** (*str*, *optional* (*default: '{data\_type}\_{pred\_name}.csv'*)) – Name of the exported files.

# export\_training\_data(filename=None)

Export all training data contained in *self.\_data*.

#### **Parameters**

**filename** (*str*, *optional* (*default:* '{*data\_type*}.*csv*')) - Name of the exported files.

### property features

Features of the input data.

Туре

numpy.ndarray

## property features\_after\_preprocessing

Features of the input data after preprocessing.

Туре

#### numpy.ndarray

# property features\_types

Types of the features.

Type

pandas.Series

# property features\_units

Units of the features.

Туре

pandas.Series

# fit()

Fit MLR model.

**Note:** Specifying keyword arguments for this function is not allowed here since *features\_after\_preprocessing* might be altered by that. Use the keyword argument fit\_kwargs during class initialization instead.

# property fit\_kwargs

Keyword arguments for fit().

Type dict

get\_ancestors(label=True, features=None, prediction\_names=None, prediction\_reference=False)

Return ancestor files.

- label (bool, optional (default: True)) Return label files.
- **features** (*list of str*, *optional* (*default: None*)) Features for which files should be returned. If None, return files for all features.

- **prediction\_names** (list of str, optional (default: None)) Prediction names for which files should be returned. If None, return files for all prediction names.
- prediction\_reference (bool, optional (default: False)) Return prediction\_reference files if available for given prediction\_names.

# Returns

Ancestor files.

# **Return type**

list of str

## Raises

**ValueError** – Invalid feature or prediction\_name given.

#### get\_data\_frame(data\_type, impute\_nans=False)

Return data frame of specified type.

### **Parameters**

- **data\_type** (*str*) Data type to be returned. Must be one of 'all', 'train' or 'test'.
- impute\_nans (bool, optional (default: False)) Impute nans if desired.

#### Returns

Desired data.

# **Return type**

pandas.DataFrame

### Raises

**TypeError** – data\_type is invalid or data does not exist (e.g. test data is not set).

### get\_x\_array(data\_type, impute\_nans=False)

Return x data of specific type.

# Parameters

- **data\_type** (*str*) Data type to be returned. Must be one of 'all', 'train' or 'test'.
- impute\_nans (bool, optional (default: False)) Impute nans if desired.

# Returns

Desired data.

# Return type

numpy.ndarray

### Raises

**TypeError** – data\_type is invalid or data does not exist (e.g. test data is not set).

# get\_y\_array(data\_type, impute\_nans=False)

Return y data of specific type.

- **data\_type** (*str*) Data type to be returned. Must be one of 'all', 'train' or 'test'.
- impute\_nans (bool, optional (default: False)) Impute nans if desired.

# Returns

Desired data.

# **Return type**

numpy.ndarray

# Raises

**TypeError** – data\_type is invalid or data does not exist (e.g. test data is not set).

### grid\_search\_cv(param\_grid, \*\*kwargs)

Perform exhaustive parameter search using cross-validation.

### **Parameters**

- **param\_grid** (*dict or list of dict*) Parameter names (keys) and ranges (values) for the search. Have to be given for each step of the pipeline separated by two underscores, i.e. s\_\_p is the parameter p for step s.
- **\*\*kwargs** (*keyword arguments, optional*) Additional options for sklearn. model\_selection.GridSearchCV.

# Raises

**ValueError** – Final regressor does not supply the attributes best\_estimator\_ or best\_params\_.

# property group\_attributes

Group attributes of the input data.

Туре

numpy.ndarray

# property label

Label of the input data.

Type str

property label\_units

Units of the label.

Туре

str

property mlr\_model\_type

MLR model type.

# Туре

str

# property numerical\_features

Numerical features.

# Туре

numpy.ndarray

## property parameters

Parameters of the complete MLR model pipeline.

Туре

dict

### plot\_1d\_model(filename=None, n\_points=1000)

Plot lineplot that represents the MLR model.

Note: This only works for a model with a single feature.

# Parameters

- **filename** (str, optional (default: '1d\_mlr\_model')) Name of the plot file.
- **n\_points** (*int*, *optional* (*default:* 1000)) Number of sampled points for the single feature (using linear spacing between minimum and maximum value).

### Raises

- sklearn.exceptions.NotFittedError MLR model is not fitted.
- ValueError MLR model is built from more than 1 feature.

### plot\_feature\_importance(filename=None, color\_coded=True)

Plot feature importance.

This function uses properties of the GBR model based on the number of appearances of that feature in the regression trees and the improvements made by the individual splits (see Friedman, 2001).

**Note:** The features plotted here are not necessarily the real input features, but the ones after preprocessing.

### **Parameters**

- filename (str, optional (default: 'feature\_importance')) Name of the plot file.
- **color\_coded** (*bool*, *optional* (*default: True*)) If True, mark positive (linear) correlations with red bars and negative (linear) correlations with blue bars. If False, all bars are blue.

#### plot\_partial\_dependences(filename=None)

Plot partial dependences for every feature.

# Parameters

```
filename (str, optional (default: 'partial_dependece_{feature}')) -
Name of the plot file.
```

# Raises

sklearn.exceptions.NotFittedError – MLR model is not fitted.

### plot\_prediction\_errors(filename=None)

Plot predicted vs. true values.

#### Parameters

**filename** (*str*, *optional* (*default: 'prediction\_errors'*)) – Name of the plot file.

# Raises

**sklearn.exceptions.NotFittedError** – MLR model is not fitted.

### plot\_residuals(filename=None)

Plot residuals of training and test (if available) data.

### Parameters

**filename** (*str*, *optional* (*default:* '*residuals*')) – Name of the plot file.

#### Raises

sklearn.exceptions.NotFittedError – MLR model is not fitted.

### plot\_residuals\_distribution(filename=None)

Plot distribution of residuals of training and test data (KDE).

# **Parameters**

**filename** (*str*, *optional* (*default:* '*residuals\_distribution*')) – Name of the plot file.

### Raises

sklearn.exceptions.NotFittedError – MLR model is not fitted.

### plot\_residuals\_histogram(filename=None)

Plot histogram of residuals of training and test data.

# Parameters

**filename** (*str*, *optional* (*default:* '*residuals\_histogram*')) - Name of the plot file.

#### Raises

sklearn.exceptions.NotFittedError – MLR model is not fitted.

### plot\_scatterplots(filename=None)

Plot scatterplots label vs. feature for every feature.

### Parameters

filename (str, optional (default: 'scatterplot\_{feature}')) - Name of
the plot file.

#### Raises

sklearn.exceptions.NotFittedError - MLR model is not fitted.

# 

Perform prediction using the MLR model(s) and write \*.nc files.

#### **Parameters**

save\_mlr\_model\_error (str or int, optional) – Additionally saves estimated squared MLR model error. This error represents the uncertainty of the prediction caused by the MLR model itself and not by errors in the prediction input data (errors in that will be considered by including datasets with var\_type set to prediction\_input\_error and setting save\_propagated\_errors to True). If the option is set to 'test', the (constant) error is estimated as RMSEP using a (hold-out) test data set. Only possible if test data is available, i.e. the option test\_size is not set to False during class initialization. If the option is set to 'logo', the (constant) error is estimated as RMSEP using the group\_attributes. Only possible if group\_datasets\_by\_attributes is given. If the option is set to an integer n (!= 0), the (constant) error is estimated as RMSEP using n-fold cross-validation.

- **save\_lime\_importance** (*bool*, *optional* (*default: False*)) Additionally saves local feature importance given by LIME (Local Interpretable Model-agnostic Explanations).
- **save\_propagated\_errors** (*bool*, *optional* (*default: False*)) Additionally saves propagated errors from prediction\_input\_error datasets. Only possible when these are available.
- **\*\*kwargs** (*keyword arguments*, *optional*) Additional options for the final regressors predict() function.

# Raises

- RuntimeError return\_var and return\_cov are both set to True.
- sklearn.exceptions.NotFittedError MLR model is not fitted.
- ValueError An invalid value for save\_mlr\_model\_error is given.
- **ValueError** save\_propagated\_errors is True and no prediction\_input\_error data is available.

## print\_correlation\_matrices()

Print correlation matrices for all datasets.

### print\_regression\_metrics(logo=False)

Print all available regression metrics for training data.

### **Parameters**

**logo** (*bool*, *optional* (*default: False*)) – Print regression metrics using sklearn.model\_selection.LeaveOneGroupOut cross-validation. Only possible when group\_datasets\_by\_attributes was given during class initialization.

# property random\_state

Random state instance.

Туре

numpy.random.RandomState

## classmethod register\_mlr\_model(mlr\_model\_type)

Add MLR model (subclass of this class) (decorator).

## reset\_pipeline()

Reset regressor pipeline.

# rfecv(\*\*kwargs)

Perform recursive feature elimination using cross-validation.

**Note:** This only works for final estimators that provide information about feature importance either through a coef\_ attribute or through a feature\_importances\_ attribute.

#### **Parameters**

```
**kwargs (keyword arguments, optional) - Additional options for sklearn. feature_selection.RFECV.
```

### Raises

**RuntimeError** – Final estimator does not provide coef\_ or feature\_importances\_ attribute.

# test\_normality\_of\_residuals()

Perform Shapiro-Wilk test to normality of residuals.

# Raises

sklearn.exceptions.NotFittedError – MLR model is not fitted.

# update\_parameters(\*\*params)

Update parameters of the whole pipeline.

**Note:** Parameter names have to be given for each step of the pipeline separated by two underscores, i.e. s\_\_p is the parameter p for step s.

#### **Parameters**

**\*\*params** (keyword arguments, optional) – Parameters for the pipeline which should be updated.

#### Raises

**ValueError** – Invalid parameter for pipeline given.

# **Base class for Linear models**

Base class for linear Machine Learning Regression models.

# Classes:

<pre>LinearModel(input_datasets, **kwargs)</pre>	Base class for linear Machine Learning models.
--	--

**class** esmvaltool.diag\_scripts.mlr.models.linear\_base.**LinearModel**(*input\_datasets*, \*\*kwargs)

Bases: MLRModel

Base class for linear Machine Learning models.

# Attributes:

categorical_features	Categorical features.
data	Input data of the MLR model.
features	Features of the input data.
features_after_preprocessing	Features of the input data after preprocessing.
features_types	Types of the features.
features_units	Units of the features.
fit_kwargs	Keyword arguments for <i>fit(</i> ).
group_attributes	Group attributes of the input data.
label	Label of the input data.
label_units	Units of the label.
mlr_model_type	MLR model type.
numerical_features	Numerical features.
parameters	Parameters of the complete MLR model pipeline.
random_state	Random state instance.

# Methods:

<pre>create(mlr_model_type, *args, **kwargs)</pre>	Create desired MLR model subclass (factory method).
efecv(**kwargs)	Perform exhaustive feature elimination using cross-validation.
<pre>export_prediction_data([filename])</pre>	Export all prediction data contained in <i>selfdata</i> .
<pre>export_training_data([filename])</pre>	Export all training data contained in <i>selfdata</i> .
fit()	Fit MLR model.
<pre>get_ancestors([label, features,])</pre>	Return ancestor files.
<pre>get_data_frame(data_type[, impute_nans])</pre>	Return data frame of specified type.
<pre>get_x_array(data_type[, impute_nans])</pre>	Return x data of specific type.
<pre>get_y_array(data_type[, impute_nans])</pre>	Return y data of specific type.
<pre>grid_search_cv(param_grid, **kwargs)</pre>	Perform exhaustive parameter search using cross-validation.
<pre>plot_1d_model([filename, n_points])</pre>	Plot lineplot that represents the MLR model.
<pre>plot_coefs([filename])</pre>	Plot linear coefficients of models.
<pre>plot_feature_importance([filename, color_coded])</pre>	Plot feature importance given by linear coefficients.
plot_partial_dependences([filename])	Plot partial dependences for every feature.
plot_prediction_errors([filename])	Plot predicted vs.
plot_residuals([filename])	Plot residuals of training and test (if available) data.
plot_residuals_distribution([filename])	Plot distribution of residuals of training and test data (KDE).
<pre>plot_residuals_histogram([filename])</pre>	Plot histogram of residuals of training and test data.
<pre>plot_scatterplots([filename])</pre>	Plot scatterplots label vs.
<pre>predict([save_mlr_model_error,])</pre>	Perform prediction using the MLR model(s) and write *.nc files.
<pre>print_correlation_matrices()</pre>	Print correlation matrices for all datasets.
<pre>print_regression_metrics([logo])</pre>	Print all available regression metrics for training data.
<pre>register_mlr_model(mlr_model_type)</pre>	Add MLR model (subclass of this class) (decorator).
reset_pipeline()	Reset regressor pipeline.
rfecv(**kwargs)	Perform recursive feature elimination using cross-validation.
<pre>test_normality_of_residuals()</pre>	Perform Shapiro-Wilk test to normality of residuals.
<pre>update_parameters(**params)</pre>	Update parameters of the whole pipeline.

# property categorical\_features

Categorical features.

# Туре

numpy.ndarray

classmethod create(mlr\_model\_type, \*args, \*\*kwargs)

Create desired MLR model subclass (factory method).

# property data

Input data of the MLR model.

Type dict

# efecv(\*\*kwargs)

Perform exhaustive feature elimination using cross-validation.

**\*\*kwargs** (*keyword arguments, optional*) – Additional options for esmvaltool. diag\_scripts.mlr. custom\_sklearn.cross\_val\_score\_weighted().

#### export\_prediction\_data(filename=None)

Export all prediction data contained in *self.\_data*.

### **Parameters**

```
filename (str, optional (default: '{data_type}_{pred_name}.csv')) -
Name of the exported files.
```

#### export\_training\_data(filename=None)

Export all training data contained in *self.\_data*.

### **Parameters**

```
filename (str, optional (default: '{data_type}.csv')) - Name of the exported files.
```

### property features

Features of the input data.

### Туре

numpy.ndarray

### property features\_after\_preprocessing

Features of the input data after preprocessing.

### Туре

numpy.ndarray

#### property features\_types

Types of the features.

#### Туре

pandas.Series

# property features\_units

Units of the features.

# Туре

pandas.Series

#### fit()

Fit MLR model.

**Note:** Specifying keyword arguments for this function is not allowed here since *features\_after\_preprocessing* might be altered by that. Use the keyword argument *fit\_kwargs* during class initialization instead.

# property fit\_kwargs

Keyword arguments for fit().

Туре

dict

get\_ancestors(label=True, features=None, prediction\_names=None, prediction\_reference=False)
Return ancestor files.

- label (bool, optional (default: True)) Return label files.
- **features** (*list of str*, *optional* (*default: None*)) Features for which files should be returned. If None, return files for all features.
- **prediction\_names** (*list of str, optional (default: None*)) Prediction names for which files should be returned. If None, return files for all prediction names.
- **prediction\_reference** (*bool*, *optional* (*default: False*)) Return prediction\_reference files if available for given prediction\_names.

### Returns

Ancestor files.

### **Return type**

list of str

# Raises

**ValueError** – Invalid feature or prediction\_name given.

### get\_data\_frame(data\_type, impute\_nans=False)

Return data frame of specified type.

### **Parameters**

- **data\_type** (*str*) Data type to be returned. Must be one of 'all', 'train' or 'test'.
- impute\_nans (bool, optional (default: False)) Impute nans if desired.

## Returns

Desired data.

# **Return type**

pandas.DataFrame

# Raises

**TypeError** – data\_type is invalid or data does not exist (e.g. test data is not set).

#### get\_x\_array(data\_type, impute\_nans=False)

Return x data of specific type.

#### Parameters

- **data\_type** (*str*) Data type to be returned. Must be one of 'all', 'train' or 'test'.
- impute\_nans (bool, optional (default: False)) Impute nans if desired.

#### Returns

Desired data.

# **Return type**

numpy.ndarray

## Raises

**TypeError** – data\_type is invalid or data does not exist (e.g. test data is not set).

#### get\_y\_array(data\_type, impute\_nans=False)

Return y data of specific type.

- **data\_type** (*str*) Data type to be returned. Must be one of 'all', 'train' or 'test'.
- impute\_nans (bool, optional (default: False)) Impute nans if desired.

#### Returns

Desired data.

# **Return type**

numpy.ndarray

# Raises

TypeError – data\_type is invalid or data does not exist (e.g. test data is not set).

#### grid\_search\_cv(param\_grid, \*\*kwargs)

Perform exhaustive parameter search using cross-validation.

## **Parameters**

- **param\_grid** (*dict or list of dict*) Parameter names (keys) and ranges (values) for the search. Have to be given for each step of the pipeline separated by two underscores, i.e. s\_\_p is the parameter p for step s.
- **\*\*kwargs** (*keyword arguments, optional*) Additional options for sklearn. model\_selection.GridSearchCV.

#### Raises

**ValueError** – Final regressor does not supply the attributes best\_estimator\_ or best\_params\_.

# property group\_attributes

Group attributes of the input data.

# Туре

numpy.ndarray

property label

Label of the input data.

Type str

property label\_units

Units of the label.

# Туре

str

property mlr\_model\_type

MLR model type.

# Туре

str

# property numerical\_features

Numerical features.

# Туре

numpy.ndarray

#### property parameters

Parameters of the complete MLR model pipeline.

Туре

# dict

```
plot_1d_model(filename=None, n_points=1000)
```

Plot lineplot that represents the MLR model.

Note: This only works for a model with a single feature.

#### **Parameters**

- **filename** (*str*, *optional* (*default:* '1d\_mlr\_model')) Name of the plot file.
- **n\_points** (*int*, *optional* (*default:* 1000)) Number of sampled points for the single feature (using linear spacing between minimum and maximum value).

#### Raises

- sklearn.exceptions.NotFittedError MLR model is not fitted.
- ValueError MLR model is built from more than 1 feature.

#### plot\_coefs(filename=None)

Plot linear coefficients of models.

Note: The features plotted here are not necessarily the real input features, but the ones after preprocessing.

# Parameters

filename (str, optional (default: 'coefs')) – Name of the plot file.

plot\_feature\_importance(filename=None, color\_coded=True)

Plot feature importance given by linear coefficients.

Note: The features plotted here are not necessarily the real input features, but the ones after preprocessing.

#### Parameters

- filename (str, optional (default: 'feature\_importance')) Name of the plot file.
- **color\_coded** (*bool*, *optional* (*default: True*)) If True, mark positive (linear) correlations with red bars and negative (linear) correlations with blue bars. If False, all bars are blue.

#### plot\_partial\_dependences(filename=None)

Plot partial dependences for every feature.

```
filename (str, optional (default: 'partial_dependece_{feature}')) -
Name of the plot file.
```

#### Raises

sklearn.exceptions.NotFittedError – MLR model is not fitted.

#### plot\_prediction\_errors(filename=None)

Plot predicted vs. true values.

# Parameters

**filename**(*str*, *optional* (*default: 'prediction\_errors'*)) – Name of the plot file.

Raises

**sklearn.exceptions.NotFittedError** – MLR model is not fitted.

## plot\_residuals(filename=None)

Plot residuals of training and test (if available) data.

# Parameters

**filename** (*str*, *optional* (*default:* '*residuals*')) – Name of the plot file.

#### Raises

sklearn.exceptions.NotFittedError – MLR model is not fitted.

#### plot\_residuals\_distribution(filename=None)

Plot distribution of residuals of training and test data (KDE).

#### **Parameters**

**filename** (*str*, *optional* (*default:* '*residuals\_distribution*')) – Name of the plot file.

#### Raises

sklearn.exceptions.NotFittedError - MLR model is not fitted.

## plot\_residuals\_histogram(filename=None)

Plot histogram of residuals of training and test data.

#### Parameters

**filename** (*str*, *optional* (*default: 'residuals\_histogram'*)) – Name of the plot file.

#### Raises

sklearn.exceptions.NotFittedError - MLR model is not fitted.

#### plot\_scatterplots(filename=None)

Plot scatterplots label vs. feature for every feature.

#### Parameters

filename (str, optional (default: 'scatterplot\_{feature}')) - Name of
the plot file.

Raises

sklearn.exceptions.NotFittedError – MLR model is not fitted.

# 

Perform prediction using the MLR model(s) and write \*.nc files.

#### **Parameters**

• **save\_mlr\_model\_error** (*str or int, optional*) – Additionally saves estimated squared MLR model error. This error represents the uncertainty of the prediction caused by the MLR model itself and not by errors in the prediction input data (errors in that will be considered by including datasets with var\_type set to prediction\_input\_error and setting save\_propagated\_errors to True). If the option is set to 'test', the (constant) error is estimated as RMSEP using a (hold-out) test data set. Only possible if test data is available, i.e. the option test\_size is not set to False during class initialization. If the option is set to 'logo', the (constant) error is estimated as RMSEP using leave-one-group-out cross-validation using the group\_attributes. Only possible if group\_datasets\_by\_attributes is given. If the option is set to an integer n (!= 0), the (constant) error is estimated as RMSEP using n-fold cross-validation.

- **save\_lime\_importance** (*bool*, *optional* (*default: False*)) Additionally saves local feature importance given by LIME (Local Interpretable Model-agnostic Explanations).
- **save\_propagated\_errors** (*bool*, *optional* (*default: False*)) Additionally saves propagated errors from prediction\_input\_error datasets. Only possible when these are available.
- **\*\*kwargs** (*keyword arguments*, *optional*) Additional options for the final regressors predict() function.

#### Raises

- RuntimeError return\_var and return\_cov are both set to True.
- sklearn.exceptions.NotFittedError MLR model is not fitted.
- ValueError An invalid value for save\_mlr\_model\_error is given.
- **ValueError** save\_propagated\_errors is True and no prediction\_input\_error data is available.

#### print\_correlation\_matrices()

Print correlation matrices for all datasets.

# print\_regression\_metrics(logo=False)

Print all available regression metrics for training data.

# **Parameters**

**logo** (bool, optional (default: False)) – Print regression metrics using sklearn.model\_selection.LeaveOneGroupOut cross-validation. Only possible when group\_datasets\_by\_attributes was given during class initialization.

# property random\_state

Random state instance.

# Туре

numpy.random.RandomState

# classmethod register\_mlr\_model(mlr\_model\_type)

Add MLR model (subclass of this class) (decorator).

# reset\_pipeline()

Reset regressor pipeline.

# rfecv(\*\*kwargs)

Perform recursive feature elimination using cross-validation.

**Note:** This only works for final estimators that provide information about feature importance either through a coef\_ attribute or through a feature\_importances\_ attribute.

# **Parameters**

```
**kwargs (keyword arguments, optional) - Additional options for sklearn. feature_selection.RFECV.
```

#### Raises

**RuntimeError** – Final estimator does not provide coef\_ or feature\_importances\_ attribute.

# test\_normality\_of\_residuals()

Perform Shapiro-Wilk test to normality of residuals.

Raises

sklearn.exceptions.NotFittedError – MLR model is not fitted.

# update\_parameters(\*\*params)

Update parameters of the whole pipeline.

**Note:** Parameter names have to be given for each step of the pipeline separated by two underscores, i.e. s\_\_p is the parameter p for step s.

#### **Parameters**

**\*\*params** (keyword arguments, optional) – Parameters for the pipeline which should be updated.

Raises

**ValueError** – Invalid parameter for pipeline given.

# 54.2.4 Available MLR models

# Gradient Boosted Regression Trees (sklearn implementation)

Gradient Boosting Regression model (using sklearn).

Use mlr\_model\_type: gbr\_sklearn to use this MLR model in the recipe.

# **Classes:**

SklearnGBRModel(input_datasets, **kwargs)	Gradient Boosting Regression model (sklearn imple-
	mentation).

class esmvaltool.diag\_scripts.mlr.models.gbr\_sklearn.SklearnGBRModel(input\_datasets, \*\*kwargs)
Bases: GBRModel

Gradient Boosting Regression model (sklearn implementation).

# Attributes:

categorical_features	Categorical features.
data	Input data of the MLR model.
features	Features of the input data.
features_after_preprocessing	Features of the input data after preprocessing.
features_types	Types of the features.
features_units	Units of the features.
fit_kwargs	Keyword arguments for fit().
group_attributes	Group attributes of the input data.
label	Label of the input data.
label_units	Units of the label.
mlr_model_type	MLR model type.
numerical_features	Numerical features.
parameters	Parameters of the complete MLR model pipeline.
random_state	Random state instance.

# Methods:

<pre>create(mlr_model_type, *args, **kwargs)</pre>	Create desired MLR model subclass (factory method).
efecv(**kwargs)	Perform exhaustive feature elimination using cross-validation.
<pre>export_prediction_data([filename])</pre>	Export all prediction data contained in <i>selfdata</i> .
<pre>export_training_data([filename])</pre>	Export all training data contained in <i>selfdata</i> .
fit()	Fit MLR model.
<pre>get_ancestors([label, features,])</pre>	Return ancestor files.
<pre>get_data_frame(data_type[, impute_nans])</pre>	Return data frame of specified type.
<pre>get_x_array(data_type[, impute_nans])</pre>	Return x data of specific type.
<pre>get_y_array(data_type[, impute_nans])</pre>	Return y data of specific type.
<pre>grid_search_cv(param_grid, **kwargs)</pre>	Perform exhaustive parameter search using cross-validation.
<pre>plot_1d_model([filename, n_points])</pre>	Plot lineplot that represents the MLR model.
<pre>plot_feature_importance([filename,</pre>	Plot feature importance.
color_coded])	
<pre>plot_partial_dependences([filename])</pre>	Plot partial dependences for every feature.
<pre>plot_prediction_errors([filename])</pre>	Plot predicted vs.
<pre>plot_residuals([filename])</pre>	Plot residuals of training and test (if available) data.
<pre>plot_residuals_distribution([filename])</pre>	Plot distribution of residuals of training and test data (KDE).
<pre>plot_residuals_histogram([filename])</pre>	Plot histogram of residuals of training and test data.
<pre>plot_scatterplots([filename])</pre>	Plot scatterplots label vs.
<pre>plot_training_progress([filename])</pre>	Plot training progress for training and (if possible) test data.
<pre>predict([save_mlr_model_error,])</pre>	Perform prediction using the MLR model(s) and write *.nc files.
<pre>print_correlation_matrices()</pre>	Print correlation matrices for all datasets.
<pre>print_regression_metrics([logo])</pre>	Print all available regression metrics for training data.
<pre>register_mlr_model(mlr_model_type)</pre>	Add MLR model (subclass of this class) (decorator).
<pre>reset_pipeline()</pre>	Reset regressor pipeline.
rfecv(**kwargs)	Perform recursive feature elimination using cross-validation.
<pre>test_normality_of_residuals()</pre>	Perform Shapiro-Wilk test to normality of residuals.
update_parameters(**params)	Update parameters of the whole pipeline.

# property categorical\_features

Categorical features.

Туре

numpy.ndarray

```
classmethod create(mlr_model_type, *args, **kwargs)
```

Create desired MLR model subclass (factory method).

# property data

Input data of the MLR model.

Туре

dict

# efecv(\*\*kwargs)

Perform exhaustive feature elimination using cross-validation.

# Parameters

```
**kwargs (keyword arguments, optional) – Additional options for esmvaltool. diag_scripts.mlr. custom_sklearn.cross_val_score_weighted().
```

#### export\_prediction\_data(filename=None)

Export all prediction data contained in *self.\_data*.

# Parameters

```
filename (str, optional (default: '{data_type}_{pred_name}.csv')) -
Name of the exported files.
```

# export\_training\_data(filename=None)

Export all training data contained in *self.\_data*.

#### **Parameters**

```
filename (str, optional (default: '{data_type}.csv')) - Name of the exported files.
```

# property features

Features of the input data.

Туре

numpy.ndarray

# property features\_after\_preprocessing

Features of the input data after preprocessing.

#### Type

numpy.ndarray

# property features\_types

Types of the features.

Туре

pandas.Series

property features\_units

Units of the features.

Туре

pandas.Series

# fit()

Fit MLR model.

**Note:** Specifying keyword arguments for this function is not allowed here since *features\_after\_preprocessing* might be altered by that. Use the keyword argument fit\_kwargs during class initialization instead.

# property fit\_kwargs

Keyword arguments for *fit(*).

# Туре

dict

get\_ancestors(label=True, features=None, prediction\_names=None, prediction\_reference=False)
Return ancestor files.

#### **Parameters**

- label (bool, optional (default: True)) Return label files.
- **features** (*list of str*, *optional* (*default: None*)) Features for which files should be returned. If None, return files for all features.
- prediction\_names (list of str, optional (default: None)) Prediction names for which files should be returned. If None, return files for all prediction names.
- **prediction\_reference** (*bool*, *optional* (*default: False*)) Return prediction\_reference files if available for given prediction\_names.

#### Returns

Ancestor files.

#### **Return type**

list of str

# Raises

**ValueError** – Invalid feature or prediction\_name given.

# get\_data\_frame(data\_type, impute\_nans=False)

Return data frame of specified type.

#### **Parameters**

- **data\_type** (*str*) Data type to be returned. Must be one of 'all', 'train' or 'test'.
- impute\_nans (bool, optional (default: False)) Impute nans if desired.

#### Returns

Desired data.

# **Return type**

pandas.DataFrame

# Raises

**TypeError** – data\_type is invalid or data does not exist (e.g. test data is not set).

#### get\_x\_array(data\_type, impute\_nans=False)

Return x data of specific type.

Parameters

- **data\_type** (*str*) Data type to be returned. Must be one of 'all', 'train' or 'test'.
- impute\_nans (bool, optional (default: False)) Impute nans if desired.

#### Returns

Desired data.

# **Return type**

numpy.ndarray

#### Raises

**TypeError** – data\_type is invalid or data does not exist (e.g. test data is not set).

#### get\_y\_array(data\_type, impute\_nans=False)

Return y data of specific type.

#### **Parameters**

- **data\_type** (*str*) Data type to be returned. Must be one of 'all', 'train' or 'test'.
- impute\_nans (bool, optional (default: False)) Impute nans if desired.

#### Returns

Desired data.

# Return type numpy.ndarray

#### Raises

**TypeError** – data\_type is invalid or data does not exist (e.g. test data is not set).

## grid\_search\_cv(param\_grid, \*\*kwargs)

Perform exhaustive parameter search using cross-validation.

#### **Parameters**

- **param\_grid** (*dict or list of dict*) Parameter names (keys) and ranges (values) for the search. Have to be given for each step of the pipeline separated by two underscores, i.e. s\_p is the parameter p for step s.
- **\*\*kwargs** (*keyword arguments, optional*) Additional options for sklearn. model\_selection.GridSearchCV.

#### Raises

**ValueError** – Final regressor does not supply the attributes best\_estimator\_ or best\_params\_.

# property group\_attributes

Group attributes of the input data.

## Туре

numpy.ndarray

# property label

Label of the input data.

Туре

str

# property label\_units

Units of the label.

Туре

str

property mlr\_model\_type

MLR model type.

Туре

str

# property numerical\_features

Numerical features.

Туре

numpy.ndarray

## property parameters

Parameters of the complete MLR model pipeline.

Type dict

# plot\_1d\_model(filename=None, n\_points=1000)

Plot lineplot that represents the MLR model.

Note: This only works for a model with a single feature.

# Parameters

- filename (str, optional (default: '1d\_mlr\_model')) Name of the plot file.
- **n\_points** (*int*, *optional* (*default:* 1000)) Number of sampled points for the single feature (using linear spacing between minimum and maximum value).

#### Raises

- sklearn.exceptions.NotFittedError MLR model is not fitted.
- ValueError MLR model is built from more than 1 feature.

#### plot\_feature\_importance(filename=None, color\_coded=True)

Plot feature importance.

This function uses properties of the GBR model based on the number of appearances of that feature in the regression trees and the improvements made by the individual splits (see Friedman, 2001).

Note: The features plotted here are not necessarily the real input features, but the ones after preprocessing.

## **Parameters**

• filename (str, optional (default: 'feature\_importance')) - Name of the plot file.

• **color\_coded** (*bool*, *optional* (*default: True*)) – If True, mark positive (linear) correlations with red bars and negative (linear) correlations with blue bars. If False, all bars are blue.

plot\_partial\_dependences(filename=None)

Plot partial dependences for every feature.

# Parameters

```
filename (str, optional (default: 'partial_dependece_{feature}')) - Name of the plot file.
```

Raises

sklearn.exceptions.NotFittedError - MLR model is not fitted.

#### plot\_prediction\_errors(filename=None)

Plot predicted vs. true values.

# Parameters

**filename** (*str*, *optional* (*default:* '*prediction\_errors*')) – Name of the plot file.

Raises

sklearn.exceptions.NotFittedError – MLR model is not fitted.

## plot\_residuals(filename=None)

Plot residuals of training and test (if available) data.

#### Parameters

**filename** (*str*, *optional* (*default:* '*residuals*')) – Name of the plot file.

#### Raises

sklearn.exceptions.NotFittedError – MLR model is not fitted.

# plot\_residuals\_distribution(filename=None)

Plot distribution of residuals of training and test data (KDE).

#### Parameters

**filename** (*str*, *optional* (*default:* '*residuals\_distribution*')) – Name of the plot file.

#### Raises

sklearn.exceptions.NotFittedError – MLR model is not fitted.

#### plot\_residuals\_histogram(filename=None)

Plot histogram of residuals of training and test data.

# Parameters

**filename** (*str*, *optional* (*default:* '*residuals\_histogram*')) – Name of the plot file.

# Raises

sklearn.exceptions.NotFittedError – MLR model is not fitted.

# plot\_scatterplots(filename=None)

Plot scatterplots label vs. feature for every feature.

# Parameters

filename (str, optional (default: 'scatterplot\_{feature}')) - Name of
the plot file.

#### Raises

sklearn.exceptions.NotFittedError – MLR model is not fitted.

#### plot\_training\_progress(filename=None)

Plot training progress for training and (if possible) test data.

#### Parameters

**filename** (*str*, *optional* (*default:* '*training\_progress*')) – Name of the plot file.

Perform prediction using the MLR model(s) and write \*.nc files.

#### Parameters

- **save\_mlr\_model\_error** (*str or int, optional*) Additionally saves estimated squared MLR model error. This error represents the uncertainty of the prediction caused by the MLR model itself and not by errors in the prediction input data (errors in that will be considered by including datasets with var\_type set to prediction\_input\_error and setting save\_propagated\_errors to True). If the option is set to 'test', the (constant) error is estimated as RMSEP using a (hold-out) test data set. Only possible if test data is available, i.e. the option test\_size is not set to False during class initialization. If the option is set to 'logo', the (constant) error is estimated as RMSEP using the group\_attributes. Only possible if group\_datasets\_by\_attributes is given. If the option is set to an integer n (!= 0), the (constant) error is estimated as RMSEP using n-fold cross-validation.
- **save\_lime\_importance** (*bool*, *optional* (*default: False*)) Additionally saves local feature importance given by LIME (Local Interpretable Model-agnostic Explanations).
- **save\_propagated\_errors** (*bool*, *optional* (*default: False*)) Additionally saves propagated errors from prediction\_input\_error datasets. Only possible when these are available.
- **\*\*kwargs** (*keyword arguments*, *optional*) Additional options for the final regressors predict() function.

## Raises

- RuntimeError return\_var and return\_cov are both set to True.
- sklearn.exceptions.NotFittedError MLR model is not fitted.
- ValueError An invalid value for save\_mlr\_model\_error is given.
- **ValueError** save\_propagated\_errors is True and no prediction\_input\_error data is available.

#### print\_correlation\_matrices()

Print correlation matrices for all datasets.

#### print\_regression\_metrics(logo=False)

Print all available regression metrics for training data.

#### Parameters

**logo** (*bool*, *optional* (*default: False*)) – Print regression metrics using sklearn.model\_selection.LeaveOneGroupOut cross-validation. Only possible when group\_datasets\_by\_attributes was given during class initialization.

# property random\_state

Random state instance.

Туре

numpy.random.RandomState

# classmethod register\_mlr\_model(mlr\_model\_type)

Add MLR model (subclass of this class) (decorator).

# reset\_pipeline()

Reset regressor pipeline.

# rfecv(\*\*kwargs)

Perform recursive feature elimination using cross-validation.

**Note:** This only works for final estimators that provide information about feature importance either through a coef\_ attribute or through a feature\_importances\_ attribute.

#### Parameters

**\*\*kwargs** (*keyword arguments, optional*) - Additional options for sklearn. feature\_selection.RFECV.

# Raises

**RuntimeError** – Final estimator does not provide coef\_ or feature\_importances\_ attribute.

#### test\_normality\_of\_residuals()

Perform Shapiro-Wilk test to normality of residuals.

#### Raises

sklearn.exceptions.NotFittedError – MLR model is not fitted.

# update\_parameters(\*\*params)

Update parameters of the whole pipeline.

**Note:** Parameter names have to be given for each step of the pipeline separated by two underscores, i.e. s\_\_p is the parameter p for step s.

# Parameters

**\*\*params** (keyword arguments, optional) – Parameters for the pipeline which should be updated.

# Raises

ValueError – Invalid parameter for pipeline given.

# Gradient Boosted Regression Trees (xgboost implementation)

Gradient Boosting Regression model (using xgboost).

Use mlr\_model\_type: gbr\_xgboost to use this MLR model in the recipe.

# **Classes:**

XGBoostGBRMode1(input_datasets, **kwargs)	Gradient Boosting Regression model (xgboost imple-
	mentation).

# class esmvaltool.diag\_scripts.mlr.models.gbr\_xgboost.XGBoostGBRModel(input\_datasets, \*\*kwargs) Bases: GBRModel

Gradient Boosting Regression model (xgboost implementation).

# Attributes:

categorical_features	Categorical features.
data	Input data of the MLR model.
features	Features of the input data.
features_after_preprocessing	Features of the input data after preprocessing.
features_types	Types of the features.
features_units	Units of the features.
fit_kwargs	Keyword arguments for fit().
group_attributes	Group attributes of the input data.
label	Label of the input data.
label_units	Units of the label.
mlr_model_type	MLR model type.
numerical_features	Numerical features.
parameters	Parameters of the complete MLR model pipeline.
random_state	Random state instance.

# Methods:

<pre>create(mlr_model_type, *args, **kwargs)</pre>	Create desired MLR model subclass (factory method).
efecv(**kwargs)	Perform exhaustive feature elimination using cross-validation.
<pre>export_prediction_data([filename])</pre>	Export all prediction data contained in <i>selfdata</i> .
<pre>export_training_data([filename])</pre>	Export all training data contained in <i>selfdata</i> .
fit()	Fit MLR model.
<pre>get_ancestors([label, features,])</pre>	Return ancestor files.
<pre>get_data_frame(data_type[, impute_nans])</pre>	Return data frame of specified type.
<pre>get_x_array(data_type[, impute_nans])</pre>	Return x data of specific type.
<pre>get_y_array(data_type[, impute_nans])</pre>	Return y data of specific type.
<pre>grid_search_cv(param_grid, **kwargs)</pre>	Perform exhaustive parameter search using cross-validation.
<pre>plot_1d_model([filename, n_points])</pre>	Plot lineplot that represents the MLR model.
<pre>plot_feature_importance([filename,</pre>	Plot feature importance.
color_coded])	
<pre>plot_partial_dependences([filename])</pre>	Plot partial dependences for every feature.
<pre>plot_prediction_errors([filename])</pre>	Plot predicted vs.
<pre>plot_residuals([filename])</pre>	Plot residuals of training and test (if available) data.
<pre>plot_residuals_distribution([filename])</pre>	Plot distribution of residuals of training and test data (KDE).
<pre>plot_residuals_histogram([filename])</pre>	Plot histogram of residuals of training and test data.
<pre>plot_scatterplots([filename])</pre>	Plot scatterplots label vs.
<pre>plot_training_progress([filename])</pre>	Plot training progress for training and (if possible) test data.
<pre>predict([save_mlr_model_error,])</pre>	Perform prediction using the MLR model(s) and write *.nc files.
<pre>print_correlation_matrices()</pre>	Print correlation matrices for all datasets.
<pre>print_regression_metrics([logo])</pre>	Print all available regression metrics for training data.
<pre>register_mlr_model(mlr_model_type)</pre>	Add MLR model (subclass of this class) (decorator).
reset_pipeline()	Reset regressor pipeline.
rfecv(**kwargs)	Perform recursive feature elimination using cross-validation.
<pre>test_normality_of_residuals()</pre>	Perform Shapiro-Wilk test to normality of residuals.
<pre>update_parameters(**params)</pre>	Update parameters of the whole pipeline.

# property categorical\_features

Categorical features.

# Туре

numpy.ndarray

classmethod create(mlr\_model\_type, \*args, \*\*kwargs)

Create desired MLR model subclass (factory method).

# property data

Input data of the MLR model.

Туре

dict

# efecv(\*\*kwargs)

Perform exhaustive feature elimination using cross-validation.

# Parameters

```
**kwargs (keyword arguments, optional) – Additional options for esmvaltool. diag_scripts.mlr. custom_sklearn.cross_val_score_weighted().
```

#### export\_prediction\_data(filename=None)

Export all prediction data contained in *self.\_data*.

# **Parameters**

**filename** (*str*, *optional* (*default:* '{*data\_type*}\_{*pred\_name*}.*csv*')) - Name of the exported files.

# export\_training\_data(filename=None)

Export all training data contained in *self.\_data*.

#### **Parameters**

**filename** (*str*, *optional* (*default:* '{*data\_type*}.*csv*')) - Name of the exported files.

# property features

Features of the input data.

#### Туре

numpy.ndarray

# property features\_after\_preprocessing

Features of the input data after preprocessing.

Туре

numpy.ndarray

# property features\_types

Types of the features.

Туре

pandas.Series

# property features\_units

Units of the features.

# Туре

pandas.Series

## fit()

Fit MLR model.

**Note:** Specifying keyword arguments for this function is not allowed here since *features\_after\_preprocessing* might be altered by that. Use the keyword argument fit\_kwargs during class initialization instead.

#### property fit\_kwargs

Keyword arguments for fit().

#### Туре

dict

get\_ancestors(label=True, features=None, prediction\_names=None, prediction\_reference=False)
Return ancestor files.

- label (bool, optional (default: True)) Return label files.
- **features** (*list of str*, *optional* (*default: None*)) Features for which files should be returned. If None, return files for all features.
- prediction\_names (list of str, optional (default: None)) Prediction names for which files should be returned. If None, return files for all prediction names.
- **prediction\_reference** (bool, optional (default: False)) Return prediction\_reference files if available for given prediction\_names.

# Returns

Ancestor files.

#### **Return type**

list of str

# Raises

**ValueError** – Invalid feature or prediction\_name given.

#### get\_data\_frame(data\_type, impute\_nans=False)

Return data frame of specified type.

#### **Parameters**

- **data\_type** (*str*) Data type to be returned. Must be one of 'all', 'train' or 'test'.
- impute\_nans (bool, optional (default: False)) Impute nans if desired.

## Returns

Desired data.

# **Return type**

pandas.DataFrame

# Raises

**TypeError** – data\_type is invalid or data does not exist (e.g. test data is not set).

#### get\_x\_array(data\_type, impute\_nans=False)

Return x data of specific type.

#### **Parameters**

- **data\_type** (*str*) Data type to be returned. Must be one of 'all', 'train' or 'test'.
- impute\_nans (bool, optional (default: False)) Impute nans if desired.

# Returns

Desired data.

# **Return type**

numpy.ndarray

# Raises

**TypeError** – data\_type is invalid or data does not exist (e.g. test data is not set).

#### get\_y\_array(data\_type, impute\_nans=False)

Return y data of specific type.

- **data\_type** (*str*) Data type to be returned. Must be one of 'all', 'train' or 'test'.
- impute\_nans (bool, optional (default: False)) Impute nans if desired.

# Returns

Desired data.

# **Return type**

numpy.ndarray

# Raises

TypeError – data\_type is invalid or data does not exist (e.g. test data is not set).

#### grid\_search\_cv(param\_grid, \*\*kwargs)

Perform exhaustive parameter search using cross-validation.

## **Parameters**

- **param\_grid** (*dict or list of dict*) Parameter names (keys) and ranges (values) for the search. Have to be given for each step of the pipeline separated by two underscores, i.e. s\_\_p is the parameter p for step s.
- **\*\*kwargs** (*keyword arguments, optional*) Additional options for sklearn. model\_selection.GridSearchCV.

#### Raises

**ValueError** – Final regressor does not supply the attributes best\_estimator\_ or best\_params\_.

# property group\_attributes

Group attributes of the input data.

# Туре

numpy.ndarray

property label

Label of the input data.

Type str

property label\_units

Units of the label.

# Туре

str

property mlr\_model\_type

MLR model type.

# Туре

str

# property numerical\_features

Numerical features.

# Туре

numpy.ndarray

#### property parameters

Parameters of the complete MLR model pipeline.

Туре

# dict

```
plot_1d_model(filename=None, n_points=1000)
```

Plot lineplot that represents the MLR model.

Note: This only works for a model with a single feature.

#### **Parameters**

- **filename** (*str*, *optional* (*default: '1d\_mlr\_model'*)) Name of the plot file.
- **n\_points** (*int*, *optional* (*default:* 1000)) Number of sampled points for the single feature (using linear spacing between minimum and maximum value).

#### Raises

- sklearn.exceptions.NotFittedError MLR model is not fitted.
- ValueError MLR model is built from more than 1 feature.

#### plot\_feature\_importance(filename=None, color\_coded=True)

Plot feature importance.

This function uses properties of the GBR model based on the number of appearances of that feature in the regression trees and the improvements made by the individual splits (see Friedman, 2001).

Note: The features plotted here are not necessarily the real input features, but the ones after preprocessing.

#### **Parameters**

- filename (str, optional (default: 'feature\_importance')) Name of the plot file.
- **color\_coded** (*bool*, *optional* (*default: True*)) If True, mark positive (linear) correlations with red bars and negative (linear) correlations with blue bars. If False, all bars are blue.

#### plot\_partial\_dependences(filename=None)

Plot partial dependences for every feature.

# Parameters

filename (str, optional (default: 'partial\_dependece\_{feature}')) Name of the plot file.

#### Raises

sklearn.exceptions.NotFittedError – MLR model is not fitted.

## plot\_prediction\_errors(filename=None)

Plot predicted vs. true values.

#### **Parameters**

**filename** (*str*, *optional* (*default:* '*prediction\_errors*')) – Name of the plot file.

#### Raises

```
sklearn.exceptions.NotFittedError – MLR model is not fitted.
```

#### plot\_residuals(filename=None)

Plot residuals of training and test (if available) data.

#### Parameters

**filename** (*str*, *optional* (*default:* '*residuals*')) – Name of the plot file.

#### Raises

sklearn.exceptions.NotFittedError – MLR model is not fitted.

#### plot\_residuals\_distribution(filename=None)

Plot distribution of residuals of training and test data (KDE).

# Parameters

**filename** (*str*, *optional* (*default:* '*residuals\_distribution*')) – Name of the plot file.

#### Raises

sklearn.exceptions.NotFittedError – MLR model is not fitted.

# plot\_residuals\_histogram(filename=None)

Plot histogram of residuals of training and test data.

# Parameters

**filename** (*str*, *optional* (*default:* '*residuals\_histogram*')) - Name of the plot file.

#### Raises

sklearn.exceptions.NotFittedError – MLR model is not fitted.

#### plot\_scatterplots(filename=None)

Plot scatterplots label vs. feature for every feature.

#### **Parameters**

filename (str, optional (default: 'scatterplot\_{feature}')) - Name of
the plot file.

#### Raises

sklearn.exceptions.NotFittedError – MLR model is not fitted.

#### plot\_training\_progress(filename=None)

Plot training progress for training and (if possible) test data.

#### Parameters

**filename** (*str*, *optional* (*default:* '*training\_progress*')) – Name of the plot file.

Perform prediction using the MLR model(s) and write \*.nc files.

#### **Parameters**

• **save\_mlr\_model\_error** (*str or int, optional*) – Additionally saves estimated squared MLR model error. This error represents the uncertainty of the prediction caused by the MLR model itself and not by errors in the prediction input data (errors in that will be considered by including datasets with var\_type set to prediction\_input\_error and setting save\_propagated\_errors to True). If the option is set to 'test', the (constant) error is estimated as RMSEP using a (hold-out) test data set. Only possible if test data is available, i.e. the option test\_size is not set to False during class initialization. If the option is set to 'logo', the (constant) error is estimated as RMSEP using leave-one-group-out cross-validation using the group\_attributes. Only possible if group\_datasets\_by\_attributes is given. If the option is set to an integer n (!= 0), the (constant) error is estimated as RMSEP using n-fold cross-validation.

- **save\_lime\_importance** (*bool*, *optional* (*default: False*)) Additionally saves local feature importance given by LIME (Local Interpretable Model-agnostic Explanations).
- **save\_propagated\_errors** (*bool*, *optional* (*default: False*)) Additionally saves propagated errors from prediction\_input\_error datasets. Only possible when these are available.
- **\*\*kwargs** (*keyword arguments*, *optional*) Additional options for the final regressors predict() function.

## Raises

- RuntimeError return\_var and return\_cov are both set to True.
- sklearn.exceptions.NotFittedError MLR model is not fitted.
- ValueError An invalid value for save\_mlr\_model\_error is given.
- **ValueError** save\_propagated\_errors is True and no prediction\_input\_error data is available.

#### print\_correlation\_matrices()

Print correlation matrices for all datasets.

#### print\_regression\_metrics(logo=False)

Print all available regression metrics for training data.

# Parameters

**logo** (bool, optional (default: False)) – Print regression metrics using sklearn.model\_selection.LeaveOneGroupOut cross-validation. Only possible when group\_datasets\_by\_attributes was given during class initialization.

# property random\_state

Random state instance.

# Туре

numpy.random.RandomState

# classmethod register\_mlr\_model(mlr\_model\_type)

Add MLR model (subclass of this class) (decorator).

# reset\_pipeline()

Reset regressor pipeline.

# rfecv(\*\*kwargs)

Perform recursive feature elimination using cross-validation.

**Note:** This only works for final estimators that provide information about feature importance either through a coef\_ attribute or through a feature\_importances\_ attribute.

# **Parameters**

```
**kwargs (keyword arguments, optional) - Additional options for sklearn. feature_selection.RFECV.
```

#### Raises

**RuntimeError** – Final estimator does not provide coef\_ or feature\_importances\_ attribute.

# test\_normality\_of\_residuals()

Perform Shapiro-Wilk test to normality of residuals.

### Raises

sklearn.exceptions.NotFittedError – MLR model is not fitted.

# update\_parameters(\*\*params)

Update parameters of the whole pipeline.

**Note:** Parameter names have to be given for each step of the pipeline separated by two underscores, i.e. s\_\_p is the parameter p for step s.

#### **Parameters**

**\*\*params** (keyword arguments, optional) – Parameters for the pipeline which should be updated.

#### Raises

**ValueError** – Invalid parameter for pipeline given.

# Gaussian Process Regression (sklearn implementation)

Gaussian Process Regression model (using sklearn).

Use mlr\_model\_type: gpr\_sklearn to use this MLR model in the recipe.

# **Classes:**

<pre>AdvancedGaussianProcessRegressor([kernel,])</pre>	Expand sklearn.gaussian_process.
	GaussianProcessRegressor.
SklearnGPRModel(input_datasets, **kwargs)	Gaussian Process Regression model (sklearn imple-
	mentation).

# class esmvaltool.diag\_scripts.mlr.models.gpr\_sklearn.AdvancedGaussianProcessRegressor(kernel=None,

\*, alpha=1e-10, optimizer='fmin\_l\_bfgs\_b n\_restarts\_optimizer= normalize\_y=False, copy\_X\_train=True, n\_targets=None, random\_state=None)

Bases: GaussianProcessRegressor

Expand sklearn.gaussian\_process.GaussianProcessRegressor.

# Methods:

<pre>fit(X, y)</pre>	Fit Gaussian process regression model.
<pre>get_metadata_routing()</pre>	Get metadata routing of this object.
<pre>get_params([deep])</pre>	Get parameters for this estimator.
<pre>log_marginal_likelihood([theta,])</pre>	Return log-marginal likelihood of theta for training
	data.
<pre>predict(x_data[, return_var, return_cov])</pre>	Expand <i>predict()</i> to accept return_var.
<pre>sample_y(X[, n_samples, random_state])</pre>	Draw samples from Gaussian process and evaluate at
	X.
<pre>score(X, y[, sample_weight])</pre>	Return the coefficient of determination of the predic-
	tion.
<pre>set_params(**params)</pre>	Set the parameters of this estimator.
<pre>set_predict_request(*[, return_cov,])</pre>	Request metadata passed to the predict method.
<pre>set_score_request(*[, sample_weight])</pre>	Request metadata passed to the score method.

# fit(X, y)

Fit Gaussian process regression model.

# **Parameters**

- **X** (array-like of shape (n\_samples, n\_features) or list of object) - Feature vectors or other representations of training data.
- **y** (array-like of shape (n\_samples,) or (n\_samples, n\_targets)) Target values.

# Returns

self – GaussianProcessRegressor class instance.

Return type object

# get\_metadata\_routing()

Get metadata routing of this object.

Please check User Guide on how the routing mechanism works.

# Returns

routing – A MetadataRequest encapsulating routing information.

# **Return type**

MetadataRequest

# get\_params(deep=True)

Get parameters for this estimator.

# Parameters

**deep** (*bool*, *default=True*) – If True, will return the parameters for this estimator and contained subobjects that are estimators.

# Returns

params – Parameter names mapped to their values.

# **Return type**

dict

# log\_marginal\_likelihood(theta=None, eval\_gradient=False, clone\_kernel=True)

Return log-marginal likelihood of theta for training data.

# Parameters

- theta (array-like of shape (n\_kernel\_params,) default=None) Kernel hyperparameters for which the log-marginal likelihood is evaluated. If None, the precomputed log\_marginal\_likelihood of self.kernel\_.theta is returned.
- **eval\_gradient** (*bool*, *default=False*) If True, the gradient of the logmarginal likelihood with respect to the kernel hyperparameters at position theta is returned additionally. If True, theta must not be None.
- **clone\_kernel** (*bool*, *default=True*) If True, the kernel attribute is copied. If False, the kernel attribute is modified, but may result in a performance improvement.

# Returns

- log\_likelihood (float) Log-marginal likelihood of theta for training data.
- **log\_likelihood\_gradient** (*ndarray of shape* (*n\_kernel\_params*,), *optional*) Gradient of the log-marginal likelihood with respect to the kernel hyperparameters at position theta. Only returned when eval\_gradient is True.

# predict(x\_data, return\_var=False, return\_cov=False)

Expand *predict()* to accept return\_var.

# sample\_y(X, n\_samples=1, random\_state=0)

Draw samples from Gaussian process and evaluate at X.

- X (array-like of shape (n\_samples\_X, n\_features) or list of object) Query points where the GP is evaluated.
- **n\_samples** (*int*, *default=1*) Number of samples drawn from the Gaussian process per query point.
- random\_state (*int*, *RandomState instance or None*, *default=0*) Determines random number generation to randomly draw samples. Pass an int for reproducible results across multiple function calls. See Glossary.

#### Returns

**y\_samples** – Values of n\_samples samples drawn from Gaussian process and evaluated at query points.

#### **Return type**

ndarray of shape (n\_samples\_X, n\_samples), or (n\_samples\_X, n\_targets, n\_samples)

score(X, y, sample\_weight=None)

Return the coefficient of determination of the prediction.

The coefficient of determination  $R^2$  is defined as  $(1-\frac{u}{v})$ , where u is the residual sum of squares ((y\_true - y\_pred)\*\* 2).sum() and v is the total sum of squares ((y\_true - y\_true.mean()) \*\* 2). sum(). The best possible score is 1.0 and it can be negative (because the model can be arbitrarily worse). A constant model that always predicts the expected value of y, disregarding the input features, would get a  $R^2$  score of 0.0.

## **Parameters**

- X (array-like of shape (n\_samples, n\_features)) Test samples. For some estimators this may be a precomputed kernel matrix or a list of generic objects instead with shape (n\_samples, n\_samples\_fitted), where n\_samples\_fitted is the number of samples used in the fitting for the estimator.
- **y** (array-like of shape (n\_samples,) or (n\_samples, n\_outputs)) True values for *X*.
- **sample\_weight** (*array-like of shape* (*n\_samples,*), *default=None*) Sample weights.

#### Returns

**score** –  $R^2$  of self.predict(X) w.r.t. y.

Return type float

#### Notes

The  $R^2$  score used when calling score on a regressor uses multioutput='uniform\_average' from version 0.23 to keep consistent with default value of r2\_score(). This influences the score method of all the multioutput regressors (except for MultiOutputRegressor).

## set\_params(\*\*params)

Set the parameters of this estimator.

The method works on simple estimators as well as on nested objects (such as Pipeline). The latter have parameters of the form <component>\_\_<parameter> so that it's possible to update each component of a nested object.

Parameters \*\*params (dict) – Estimator parameters.

**Returns self** – Estimator instance.

Return type estimator instance

 $set\_predict\_request(*, return\_cov: bool | None | str = '$UNCHANGED$', return\_var: bool | None | str = '$UNCHANGED$', x_data: bool | None | str = '$UNCHANGED$') \rightarrow AdvancedGaussianProcessRegressor$ 

Request metadata passed to the predict method.

Note that this method is only relevant if enable\_metadata\_routing=True (see sklearn. set\_config()). Please see User Guide on how the routing mechanism works.

The options for each parameter are:

- True: metadata is requested, and passed to predict if provided. The request is ignored if metadata is not provided.
- False: metadata is not requested and the meta-estimator will not pass it to predict.
- None: metadata is not requested, and the meta-estimator will raise an error if the user provides it.
- str: metadata should be passed to the meta-estimator with this given alias instead of the original name.

The default (sklearn.utils.metadata\_routing.UNCHANGED) retains the existing request. This allows you to change the request for some parameters and not others.

Added in version 1.3.

**Note:** This method is only relevant if this estimator is used as a sub-estimator of a meta-estimator, e.g. used inside a Pipeline. Otherwise it has no effect.

#### **Parameters**

- return\_cov (str, True, False, or None, default=sklearn.utils. metadata\_routing.UNCHANGED) – Metadata routing for return\_cov parameter in predict.
- return\_var (str, True, False, or None, default=sklearn.utils. metadata\_routing.UNCHANGED) - Metadata routing for return\_var parameter in predict.
- **x\_data** (str, True, False, or None, default=sklearn.utils. metadata\_routing.UNCHANGED) - Metadata routing for x\_data parameter in predict.

#### Returns

self – The updated object.

# **Return type**

object

# set\_score\_request(\*, sample\_weight: bool | None | $str = '$UNCHANGED$') \rightarrow AdvancedGaussianProcessRegressor$

Request metadata passed to the score method.

Note that this method is only relevant if enable\_metadata\_routing=True (see sklearn. set\_config()). Please see User Guide on how the routing mechanism works.

The options for each parameter are:

- True: metadata is requested, and passed to score if provided. The request is ignored if metadata is not provided.
- False: metadata is not requested and the meta-estimator will not pass it to score.
- None: metadata is not requested, and the meta-estimator will raise an error if the user provides it.

• str: metadata should be passed to the meta-estimator with this given alias instead of the original name.

The default (sklearn.utils.metadata\_routing.UNCHANGED) retains the existing request. This allows you to change the request for some parameters and not others.

Added in version 1.3.

**Note:** This method is only relevant if this estimator is used as a sub-estimator of a meta-estimator, e.g. used inside a **Pipeline**. Otherwise it has no effect.

# Parameters

sample\_weight (str, True, False, or None, default=sklearn.utils. metadata\_routing.UNCHANGED) - Metadata routing for sample\_weight parameter in score.

# Returns

self – The updated object.

# **Return type**

object

# class esmvaltool.diag\_scripts.mlr.models.gpr\_sklearn.SklearnGPRModel(input\_datasets, \*\*kwargs) Bases: MLRModel

Gaussian Process Regression model (sklearn implementation).

# Attributes:

categorical_features	Categorical features.
data	Input data of the MLR model.
features	Features of the input data.
features_after_preprocessing	Features of the input data after preprocessing.
features_types	Types of the features.
features_units	Units of the features.
fit_kwargs	Keyword arguments for <i>fit(</i> ).
group_attributes	Group attributes of the input data.
label	Label of the input data.
label_units	Units of the label.
mlr_model_type	MLR model type.
numerical_features	Numerical features.
parameters	Parameters of the complete MLR model pipeline.
random_state	Random state instance.

# Methods:

<pre>create(mlr_model_type, *args, **kwargs)</pre>	Create desired MLR model subclass (factory method).
efecv(**kwargs)	Perform exhaustive feature elimination using cross-validation.
<pre>export_prediction_data([filename])</pre>	Export all prediction data contained in <i>selfdata</i> .
<pre>export_training_data([filename])</pre>	Export all training data contained in <i>selfdata</i> .
fit()	Fit MLR model.
<pre>get_ancestors([label, features,])</pre>	Return ancestor files.
<pre>get_data_frame(data_type[, impute_nans])</pre>	Return data frame of specified type.
<pre>get_x_array(data_type[, impute_nans])</pre>	Return x data of specific type.
<pre>get_y_array(data_type[, impute_nans])</pre>	Return y data of specific type.
<pre>grid_search_cv(param_grid, **kwargs)</pre>	Perform exhaustive parameter search using cross-validation.
<pre>plot_1d_model([filename, n_points])</pre>	Plot lineplot that represents the MLR model.
<pre>plot_partial_dependences([filename])</pre>	Plot partial dependences for every feature.
<pre>plot_prediction_errors([filename])</pre>	Plot predicted vs.
<pre>plot_residuals([filename])</pre>	Plot residuals of training and test (if available) data.
<pre>plot_residuals_distribution([filename])</pre>	Plot distribution of residuals of training and test data (KDE).
<pre>plot_residuals_histogram([filename])</pre>	Plot histogram of residuals of training and test data.
<pre>plot_scatterplots([filename])</pre>	Plot scatterplots label vs.
<pre>predict([save_mlr_model_error,])</pre>	Perform prediction using the MLR model(s) and write *.nc files.
<pre>print_correlation_matrices()</pre>	Print correlation matrices for all datasets.
<pre>print_kernel_info()</pre>	Print information of the fitted kernel of the GPR model.
<pre>print_regression_metrics([logo])</pre>	Print all available regression metrics for training data.
<pre>register_mlr_model(mlr_model_type)</pre>	Add MLR model (subclass of this class) (decorator).
reset_pipeline()	Reset regressor pipeline.
rfecv(**kwargs)	Perform recursive feature elimination using cross-validation.
<pre>test_normality_of_residuals()</pre>	Perform Shapiro-Wilk test to normality of residuals.
update_parameters(**params)	Update parameters of the whole pipeline.

# property categorical\_features

Categorical features.

## Туре

# numpy.ndarray

classmethod create(mlr\_model\_type, \*args, \*\*kwargs)

 $Create \ desired \ MLR \ model \ subclass \ (factory \ method).$ 

# property data

Input data of the MLR model.

Туре

dict

# efecv(\*\*kwargs)

Perform exhaustive feature elimination using cross-validation.

```
**kwargs (keyword arguments, optional) – Additional options for esmvaltool. diag_scripts.mlr. custom_sklearn.cross_val_score_weighted().
```

# export\_prediction\_data(filename=None)

Export all prediction data contained in *self.\_data*.

# Parameters

**filename** (*str*, *optional* (*default: '{data\_type}\_{pred\_name}.csv'*)) – Name of the exported files.

# export\_training\_data(filename=None)

Export all training data contained in *self.\_data*.

#### **Parameters**

**filename** (*str*, *optional* (*default:* '{*data\_type*}.*csv*')) - Name of the exported files.

#### property features

Features of the input data.

Туре

numpy.ndarray

# property features\_after\_preprocessing

Features of the input data after preprocessing.

Туре

#### numpy.ndarray

# property features\_types

Types of the features.

Type

pandas.Series

# property features\_units

Units of the features.

Туре

pandas.Series

# fit()

Fit MLR model.

**Note:** Specifying keyword arguments for this function is not allowed here since *features\_after\_preprocessing* might be altered by that. Use the keyword argument fit\_kwargs during class initialization instead.

# property fit\_kwargs

Keyword arguments for fit().

Type dict

get\_ancestors(label=True, features=None, prediction\_names=None, prediction\_reference=False)

Return ancestor files.

- label (bool, optional (default: True)) Return label files.
- **features** (*list of str*, *optional* (*default: None*)) Features for which files should be returned. If None, return files for all features.

- **prediction\_names** (list of str, optional (default: None)) Prediction names for which files should be returned. If None, return files for all prediction names.
- prediction\_reference (bool, optional (default: False)) Return prediction\_reference files if available for given prediction\_names.

# Returns

Ancestor files.

# **Return type**

list of str

# Raises

**ValueError** – Invalid feature or prediction\_name given.

#### get\_data\_frame(data\_type, impute\_nans=False)

Return data frame of specified type.

#### **Parameters**

- **data\_type** (*str*) Data type to be returned. Must be one of 'all', 'train' or 'test'.
- impute\_nans (bool, optional (default: False)) Impute nans if desired.

#### Returns

Desired data.

# **Return type**

pandas.DataFrame

#### Raises

**TypeError** – data\_type is invalid or data does not exist (e.g. test data is not set).

#### get\_x\_array(data\_type, impute\_nans=False)

Return x data of specific type.

# Parameters

- **data\_type** (*str*) Data type to be returned. Must be one of 'all', 'train' or 'test'.
- impute\_nans (bool, optional (default: False)) Impute nans if desired.

# Returns

Desired data.

# **Return type**

numpy.ndarray

#### Raises

**TypeError** – data\_type is invalid or data does not exist (e.g. test data is not set).

# get\_y\_array(data\_type, impute\_nans=False)

Return y data of specific type.

- **data\_type** (*str*) Data type to be returned. Must be one of 'all', 'train' or 'test'.
- impute\_nans (bool, optional (default: False)) Impute nans if desired.

# Returns

Desired data.

# **Return type**

numpy.ndarray

# Raises

**TypeError** – data\_type is invalid or data does not exist (e.g. test data is not set).

#### grid\_search\_cv(param\_grid, \*\*kwargs)

Perform exhaustive parameter search using cross-validation.

#### **Parameters**

- **param\_grid** (*dict or list of dict*) Parameter names (keys) and ranges (values) for the search. Have to be given for each step of the pipeline separated by two underscores, i.e. s\_\_p is the parameter p for step s.
- **\*\*kwargs** (*keyword arguments, optional*) Additional options for sklearn. model\_selection.GridSearchCV.

# Raises

**ValueError** – Final regressor does not supply the attributes best\_estimator\_ or best\_params\_.

# property group\_attributes

Group attributes of the input data.

Туре

numpy.ndarray

# property label

Label of the input data.

Type str

property label\_units

Units of the label.

Туре

str

property mlr\_model\_type

MLR model type.

# Туре

str

# property numerical\_features

Numerical features.

# Туре

numpy.ndarray

# property parameters

Parameters of the complete MLR model pipeline.

Туре

dict

#### plot\_1d\_model(filename=None, n\_points=1000)

Plot lineplot that represents the MLR model.

**Note:** This only works for a model with a single feature.

# Parameters

- **filename** (*str*, *optional* (*default: '1d\_mlr\_model'*)) Name of the plot file.
- **n\_points** (*int*, *optional* (*default:* 1000)) Number of sampled points for the single feature (using linear spacing between minimum and maximum value).

#### Raises

- sklearn.exceptions.NotFittedError MLR model is not fitted.
- ValueError MLR model is built from more than 1 feature.

#### plot\_partial\_dependences(filename=None)

Plot partial dependences for every feature.

# Parameters

filename (str, optional (default: 'partial\_dependece\_{feature}')) Name of the plot file.

#### Raises

sklearn.exceptions.NotFittedError - MLR model is not fitted.

# plot\_prediction\_errors(filename=None)

Plot predicted vs. true values.

# Parameters

**filename** (*str*, *optional* (*default: 'prediction\_errors'*)) – Name of the plot file.

#### Raises

sklearn.exceptions.NotFittedError – MLR model is not fitted.

#### plot\_residuals(filename=None)

Plot residuals of training and test (if available) data.

# Parameters

**filename** (*str*, *optional* (*default:* '*residuals*')) – Name of the plot file.

#### Raises

sklearn.exceptions.NotFittedError – MLR model is not fitted.

# plot\_residuals\_distribution(filename=None)

Plot distribution of residuals of training and test data (KDE).

#### **Parameters**

**filename** (*str*, *optional* (*default: 'residuals\_distribution'*)) – Name of the plot file.

#### Raises

sklearn.exceptions.NotFittedError – MLR model is not fitted.

#### plot\_residuals\_histogram(filename=None)

Plot histogram of residuals of training and test data.

#### Parameters

**filename** (*str*, *optional* (*default: 'residuals\_histogram'*)) – Name of the plot file.

#### Raises

sklearn.exceptions.NotFittedError – MLR model is not fitted.

#### plot\_scatterplots(filename=None)

Plot scatterplots label vs. feature for every feature.

#### Parameters

**filename** (*str*, *optional* (*default:* '*scatterplot\_{feature}*')) – Name of the plot file.

#### Raises

#### sklearn.exceptions.NotFittedError – MLR model is not fitted.

Perform prediction using the MLR model(s) and write \*.nc files.

#### **Parameters**

- save\_mlr\_model\_error (str or int, optional) Additionally saves estimated squared MLR model error. This error represents the uncertainty of the prediction caused by the MLR model itself and not by errors in the prediction input data (errors in that will be considered by including datasets with var\_type set to prediction\_input\_error and setting save\_propagated\_errors to True). If the option is set to 'test', the (constant) error is estimated as RMSEP using a (hold-out) test data set. Only possible if test data is available, i.e. the option test\_size is not set to False during class initialization. If the option is set to 'logo', the (constant) error is estimated as RMSEP using the group\_attributes. Only possible if group\_datasets\_by\_attributes is given. If the option is set to an integer n (!= 0), the (constant) error is estimated as RMSEP using n-fold cross-validation.
- **save\_lime\_importance** (*bool*, *optional* (*default: False*)) Additionally saves local feature importance given by LIME (Local Interpretable Model-agnostic Explanations).
- **save\_propagated\_errors** (*bool*, *optional* (*default: False*)) Additionally saves propagated errors from prediction\_input\_error datasets. Only possible when these are available.
- **\*\*kwargs** (*keyword arguments*, *optional*) Additional options for the final regressors predict() function.

#### Raises

- **RuntimeError** return\_var and return\_cov are both set to True.
- sklearn.exceptions.NotFittedError MLR model is not fitted.
- ValueError An invalid value for save\_mlr\_model\_error is given.
- **ValueError** save\_propagated\_errors is True and no prediction\_input\_error data is available.

#### print\_correlation\_matrices()

Print correlation matrices for all datasets.

# print\_kernel\_info()

Print information of the fitted kernel of the GPR model.

#### print\_regression\_metrics(logo=False)

Print all available regression metrics for training data.

# Parameters

**logo** (bool, optional (default: False)) – Print regression metrics using sklearn.model\_selection.LeaveOneGroupOut cross-validation. Only possible when group\_datasets\_by\_attributes was given during class initialization.

# property random\_state

Random state instance.

#### Type

numpy.random.RandomState

#### classmethod register\_mlr\_model(mlr\_model\_type)

Add MLR model (subclass of this class) (decorator).

# reset\_pipeline()

Reset regressor pipeline.

# rfecv(\*\*kwargs)

Perform recursive feature elimination using cross-validation.

**Note:** This only works for final estimators that provide information about feature importance either through a coef\_ attribute or through a feature\_importances\_ attribute.

#### Parameters

**\*\*kwargs** (*keyword arguments, optional*) - Additional options for sklearn. feature\_selection.RFECV.

#### Raises

**RuntimeError** – Final estimator does not provide coef\_ or feature\_importances\_ attribute.

#### test\_normality\_of\_residuals()

Perform Shapiro-Wilk test to normality of residuals.

#### Raises

sklearn.exceptions.NotFittedError - MLR model is not fitted.

# update\_parameters(\*\*params)

Update parameters of the whole pipeline.

**Note:** Parameter names have to be given for each step of the pipeline separated by two underscores, i.e. s\_\_p is the parameter p for step s.

#### Parameters

**\*\*params** (keyword arguments, optional) – Parameters for the pipeline which should be updated.

Raises

**ValueError** – Invalid parameter for pipeline given.

# **Huber Regression**

Huber Regression model.

Use mlr\_model\_type: huber to use this MLR model in the recipe.

# Classes:

HuberRegressionModel(input	datasets, **kwargs)	Huber Regression model.	

# class esmvaltool.diag\_scripts.mlr.models.huber.HuberRegressionModel(input\_datasets, \*\*kwargs) Bases: LinearModel

Huber Regression model.

# Attributes:

categorical_features	Categorical features.
data	Input data of the MLR model.
features	Features of the input data.
features_after_preprocessing	Features of the input data after preprocessing.
features_types	Types of the features.
features_units	Units of the features.
fit_kwargs	Keyword arguments for <i>fit(</i> ).
group_attributes	Group attributes of the input data.
label	Label of the input data.
label_units	Units of the label.
mlr_model_type	MLR model type.
numerical_features	Numerical features.
parameters	Parameters of the complete MLR model pipeline.
random_state	Random state instance.

# Methods:

<pre>create(mlr_model_type, *args, **kwargs)</pre>	Create desired MLR model subclass (factory method).
efecv(**kwargs)	Perform exhaustive feature elimination using cross-validation.
<pre>export_prediction_data([filename])</pre>	Export all prediction data contained in <i>selfdata</i> .
<pre>export_training_data([filename])</pre>	Export all training data contained in <i>selfdata</i> .
fit()	Fit MLR model.
<pre>get_ancestors([label, features,])</pre>	Return ancestor files.
<pre>get_data_frame(data_type[, impute_nans])</pre>	Return data frame of specified type.
<pre>get_x_array(data_type[, impute_nans])</pre>	Return x data of specific type.
<pre>get_y_array(data_type[, impute_nans])</pre>	Return y data of specific type.
<pre>grid_search_cv(param_grid, **kwargs)</pre>	Perform exhaustive parameter search using cross-validation.
<pre>plot_1d_model([filename, n_points])</pre>	Plot lineplot that represents the MLR model.
<pre>plot_coefs([filename])</pre>	Plot linear coefficients of models.
<pre>plot_feature_importance([filename, color_coded])</pre>	Plot feature importance given by linear coefficients.
plot_partial_dependences([filename])	Plot partial dependences for every feature.
plot_prediction_errors([filename])	Plot predicted vs.
plot_residuals([filename])	Plot residuals of training and test (if available) data.
plot_residuals_distribution([filename])	Plot distribution of residuals of training and test data
	(KDE).
<pre>plot_residuals_histogram([filename])</pre>	Plot histogram of residuals of training and test data.
<pre>plot_scatterplots([filename])</pre>	Plot scatterplots label vs.
<pre>predict([save_mlr_model_error,])</pre>	Perform prediction using the MLR model(s) and write *.nc files.
<pre>print_correlation_matrices()</pre>	Print correlation matrices for all datasets.
<pre>print_regression_metrics([logo])</pre>	Print all available regression metrics for training data.
<pre>register_mlr_model(mlr_model_type)</pre>	Add MLR model (subclass of this class) (decorator).
reset_pipeline()	Reset regressor pipeline.
rfecv(**kwargs)	Perform recursive feature elimination using cross-validation.
<pre>test_normality_of_residuals()</pre>	Perform Shapiro-Wilk test to normality of residuals.
<pre>update_parameters(**params)</pre>	Update parameters of the whole pipeline.

# property categorical\_features

Categorical features.

# Туре

numpy.ndarray

classmethod create(mlr\_model\_type, \*args, \*\*kwargs)

Create desired MLR model subclass (factory method).

# property data

Input data of the MLR model.

Type dict

# efecv(\*\*kwargs)

Perform exhaustive feature elimination using cross-validation.

**\*\*kwargs** (*keyword arguments, optional*) – Additional options for esmvaltool. diag\_scripts.mlr. custom\_sklearn.cross\_val\_score\_weighted().

#### export\_prediction\_data(filename=None)

Export all prediction data contained in *self.\_data*.

### **Parameters**

```
filename (str, optional (default: '{data_type}_{pred_name}.csv')) -
Name of the exported files.
```

#### export\_training\_data(filename=None)

Export all training data contained in *self.\_data*.

### **Parameters**

```
filename (str, optional (default: '{data_type}.csv')) - Name of the exported files.
```

### property features

Features of the input data.

#### Туре

numpy.ndarray

### property features\_after\_preprocessing

Features of the input data after preprocessing.

### Туре

numpy.ndarray

#### property features\_types

Types of the features.

#### Туре

pandas.Series

# property features\_units

Units of the features.

# Туре

pandas.Series

#### fit()

Fit MLR model.

**Note:** Specifying keyword arguments for this function is not allowed here since *features\_after\_preprocessing* might be altered by that. Use the keyword argument *fit\_kwargs* during class initialization instead.

# property fit\_kwargs

Keyword arguments for fit().

Туре

dict

get\_ancestors(label=True, features=None, prediction\_names=None, prediction\_reference=False)
Return ancestor files.

- label (bool, optional (default: True)) Return label files.
- **features** (*list of str*, *optional* (*default: None*)) Features for which files should be returned. If None, return files for all features.
- **prediction\_names** (*list of str, optional (default: None*)) Prediction names for which files should be returned. If None, return files for all prediction names.
- **prediction\_reference** (*bool*, *optional* (*default: False*)) Return prediction\_reference files if available for given prediction\_names.

### Returns

Ancestor files.

#### **Return type**

list of str

# Raises

ValueError – Invalid feature or prediction\_name given.

### get\_data\_frame(data\_type, impute\_nans=False)

Return data frame of specified type.

### **Parameters**

- **data\_type** (*str*) Data type to be returned. Must be one of 'all', 'train' or 'test'.
- impute\_nans (bool, optional (default: False)) Impute nans if desired.

# Returns

Desired data.

# **Return type**

pandas.DataFrame

# Raises

**TypeError** – data\_type is invalid or data does not exist (e.g. test data is not set).

#### get\_x\_array(data\_type, impute\_nans=False)

Return x data of specific type.

#### Parameters

- **data\_type** (*str*) Data type to be returned. Must be one of 'all', 'train' or 'test'.
- impute\_nans (bool, optional (default: False)) Impute nans if desired.

#### Returns

Desired data.

# **Return type**

numpy.ndarray

# Raises

**TypeError** – data\_type is invalid or data does not exist (e.g. test data is not set).

#### get\_y\_array(data\_type, impute\_nans=False)

Return y data of specific type.

- **data\_type** (*str*) Data type to be returned. Must be one of 'all', 'train' or 'test'.
- impute\_nans (bool, optional (default: False)) Impute nans if desired.

### Returns

Desired data.

# **Return type**

numpy.ndarray

# Raises

TypeError – data\_type is invalid or data does not exist (e.g. test data is not set).

### grid\_search\_cv(param\_grid, \*\*kwargs)

Perform exhaustive parameter search using cross-validation.

## **Parameters**

- **param\_grid** (*dict or list of dict*) Parameter names (keys) and ranges (values) for the search. Have to be given for each step of the pipeline separated by two underscores, i.e. s\_\_p is the parameter p for step s.
- **\*\*kwargs** (*keyword arguments, optional*) Additional options for sklearn. model\_selection.GridSearchCV.

#### Raises

**ValueError** – Final regressor does not supply the attributes best\_estimator\_ or best\_params\_.

# property group\_attributes

Group attributes of the input data.

# Туре

numpy.ndarray

property label

Label of the input data.

Type str

property label\_units

Units of the label.

# Туре

str

# property mlr\_model\_type

MLR model type.

# Туре

str

# property numerical\_features

Numerical features.

# Туре

numpy.ndarray

#### property parameters

Parameters of the complete MLR model pipeline.

Туре

# dict

```
plot_1d_model(filename=None, n_points=1000)
```

Plot lineplot that represents the MLR model.

Note: This only works for a model with a single feature.

### **Parameters**

- **filename** (*str*, *optional* (*default:* '1d\_mlr\_model')) Name of the plot file.
- **n\_points** (*int*, *optional* (*default:* 1000)) Number of sampled points for the single feature (using linear spacing between minimum and maximum value).

#### Raises

- sklearn.exceptions.NotFittedError MLR model is not fitted.
- ValueError MLR model is built from more than 1 feature.

### plot\_coefs(filename=None)

Plot linear coefficients of models.

Note: The features plotted here are not necessarily the real input features, but the ones after preprocessing.

# Parameters

filename (str, optional (default: 'coefs')) – Name of the plot file.

plot\_feature\_importance(filename=None, color\_coded=True)

Plot feature importance given by linear coefficients.

Note: The features plotted here are not necessarily the real input features, but the ones after preprocessing.

### **Parameters**

- filename (str, optional (default: 'feature\_importance')) Name of the plot file.
- **color\_coded** (*bool*, *optional* (*default: True*)) If True, mark positive (linear) correlations with red bars and negative (linear) correlations with blue bars. If False, all bars are blue.

### plot\_partial\_dependences(filename=None)

Plot partial dependences for every feature.

```
filename (str, optional (default: 'partial_dependece_{feature}')) -
Name of the plot file.
```

#### Raises

sklearn.exceptions.NotFittedError – MLR model is not fitted.

### plot\_prediction\_errors(filename=None)

Plot predicted vs. true values.

# Parameters

**filename**(*str*, *optional* (*default: 'prediction\_errors'*)) – Name of the plot file.

Raises

**sklearn.exceptions.NotFittedError** – MLR model is not fitted.

# plot\_residuals(filename=None)

Plot residuals of training and test (if available) data.

# Parameters

**filename** (*str*, *optional* (*default:* '*residuals*')) – Name of the plot file.

#### Raises

sklearn.exceptions.NotFittedError – MLR model is not fitted.

### plot\_residuals\_distribution(filename=None)

Plot distribution of residuals of training and test data (KDE).

#### **Parameters**

**filename** (*str*, *optional* (*default:* '*residuals\_distribution*')) – Name of the plot file.

#### Raises

sklearn.exceptions.NotFittedError - MLR model is not fitted.

## plot\_residuals\_histogram(filename=None)

Plot histogram of residuals of training and test data.

#### Parameters

**filename** (*str*, *optional* (*default: 'residuals\_histogram'*)) – Name of the plot file.

#### Raises

sklearn.exceptions.NotFittedError - MLR model is not fitted.

### plot\_scatterplots(filename=None)

Plot scatterplots label vs. feature for every feature.

#### Parameters

filename (str, optional (default: 'scatterplot\_{feature}')) - Name of
the plot file.

Raises

sklearn.exceptions.NotFittedError – MLR model is not fitted.

# 

Perform prediction using the MLR model(s) and write \*.nc files.

#### **Parameters**

• **save\_mlr\_model\_error** (*str or int, optional*) – Additionally saves estimated squared MLR model error. This error represents the uncertainty of the prediction caused by the MLR model itself and not by errors in the prediction input data (errors in that will be considered by including datasets with var\_type set to prediction\_input\_error and setting save\_propagated\_errors to True). If the option is set to 'test', the (constant) error is estimated as RMSEP using a (hold-out) test data set. Only possible if test data is available, i.e. the option test\_size is not set to False during class initialization. If the option is set to 'logo', the (constant) error is estimated as RMSEP using leave-one-group-out cross-validation using the group\_attributes. Only possible if group\_datasets\_by\_attributes is given. If the option is set to an integer n (!= 0), the (constant) error is estimated as RMSEP using n-fold cross-validation.

- **save\_lime\_importance** (*bool*, *optional* (*default: False*)) Additionally saves local feature importance given by LIME (Local Interpretable Model-agnostic Explanations).
- **save\_propagated\_errors** (*bool*, *optional* (*default: False*)) Additionally saves propagated errors from prediction\_input\_error datasets. Only possible when these are available.
- **\*\*kwargs** (*keyword arguments*, *optional*) Additional options for the final regressors predict() function.

### Raises

- RuntimeError return\_var and return\_cov are both set to True.
- sklearn.exceptions.NotFittedError MLR model is not fitted.
- ValueError An invalid value for save\_mlr\_model\_error is given.
- **ValueError** save\_propagated\_errors is True and no prediction\_input\_error data is available.

### print\_correlation\_matrices()

Print correlation matrices for all datasets.

### print\_regression\_metrics(logo=False)

Print all available regression metrics for training data.

# **Parameters**

**logo** (bool, optional (default: False)) – Print regression metrics using sklearn.model\_selection.LeaveOneGroupOut cross-validation. Only possible when group\_datasets\_by\_attributes was given during class initialization.

# property random\_state

Random state instance.

# Туре

numpy.random.RandomState

# classmethod register\_mlr\_model(mlr\_model\_type)

Add MLR model (subclass of this class) (decorator).

# reset\_pipeline()

Reset regressor pipeline.

# rfecv(\*\*kwargs)

Perform recursive feature elimination using cross-validation.

**Note:** This only works for final estimators that provide information about feature importance either through a coef\_ attribute or through a feature\_importances\_ attribute.

# **Parameters**

```
**kwargs (keyword arguments, optional) - Additional options for sklearn. feature_selection.RFECV.
```

### Raises

**RuntimeError** – Final estimator does not provide coef\_ or feature\_importances\_ attribute.

# test\_normality\_of\_residuals()

Perform Shapiro-Wilk test to normality of residuals.

## Raises

sklearn.exceptions.NotFittedError – MLR model is not fitted.

# update\_parameters(\*\*params)

Update parameters of the whole pipeline.

**Note:** Parameter names have to be given for each step of the pipeline separated by two underscores, i.e. s\_\_p is the parameter p for step s.

#### **Parameters**

**\*\*params** (keyword arguments, optional) – Parameters for the pipeline which should be updated.

### Raises

**ValueError** – Invalid parameter for pipeline given.

# **Kernel Ridge Regression**

Kernel Ridge Regression model.

Use mlr\_model\_type: krr to use this MLR model in the recipe.

# **Classes:**

*KRRModel*(input\_datasets, \*\*kwargs) Kernel Ridge Regression model.

class esmvaltool.diag\_scripts.mlr.models.krr.KRRModel(input\_datasets, \*\*kwargs)

Bases: MLRModel

Kernel Ridge Regression model.

Attributes:

categorical_features	Categorical features.
data	Input data of the MLR model.
features	Features of the input data.
features_after_preprocessing	Features of the input data after preprocessing.
features_types	Types of the features.
features_units	Units of the features.
fit_kwargs	Keyword arguments for fit().
group_attributes	Group attributes of the input data.
label	Label of the input data.
label_units	Units of the label.
mlr_model_type	MLR model type.
numerical_features	Numerical features.
parameters	Parameters of the complete MLR model pipeline.
random_state	Random state instance.

# Methods:

<pre>create(mlr_model_type, *args, **kwargs)</pre>	Create desired MLR model subclass (factory method).
efecv(**kwargs)	Perform exhaustive feature elimination using cross- validation.
amont prediction data([flamoma])	
export_prediction_data([filename])	Export all prediction data contained in <i>selfdata</i> .
<pre>export_training_data([filename])</pre>	Export all training data contained in <i>selfdata</i> .
fit()	Fit MLR model.
<pre>get_ancestors([label, features,])</pre>	Return ancestor files.
<pre>get_data_frame(data_type[, impute_nans])</pre>	Return data frame of specified type.
<pre>get_x_array(data_type[, impute_nans])</pre>	Return x data of specific type.
<pre>get_y_array(data_type[, impute_nans])</pre>	Return y data of specific type.
<pre>grid_search_cv(param_grid, **kwargs)</pre>	Perform exhaustive parameter search using cross-validation.
<pre>plot_1d_model([filename, n_points])</pre>	Plot lineplot that represents the MLR model.
<pre>plot_partial_dependences([filename])</pre>	Plot partial dependences for every feature.
<pre>plot_prediction_errors([filename])</pre>	Plot predicted vs.
<pre>plot_residuals([filename])</pre>	Plot residuals of training and test (if available) data.
<pre>plot_residuals_distribution([filename])</pre>	Plot distribution of residuals of training and test data (KDE).
<pre>plot_residuals_histogram([filename])</pre>	Plot histogram of residuals of training and test data.
<pre>plot_scatterplots([filename])</pre>	Plot scatterplots label vs.
<pre>predict([save_mlr_model_error,])</pre>	Perform prediction using the MLR model(s) and write *.nc files.
<pre>print_correlation_matrices()</pre>	Print correlation matrices for all datasets.
<pre>print_regression_metrics([logo])</pre>	Print all available regression metrics for training data.
<pre>register_mlr_model(mlr_model_type)</pre>	Add MLR model (subclass of this class) (decorator).
reset_pipeline()	Reset regressor pipeline.
rfecv(**kwargs)	Perform recursive feature elimination using cross-validation.
<pre>test_normality_of_residuals()</pre>	Perform Shapiro-Wilk test to normality of residuals.
update_parameters(**params)	Update parameters of the whole pipeline.

# property categorical\_features

Categorical features.

# Туре

numpy.ndarray

# classmethod create(mlr\_model\_type, \*args, \*\*kwargs)

Create desired MLR model subclass (factory method).

# property data

Input data of the MLR model.

## Type

dict

# efecv(\*\*kwargs)

Perform exhaustive feature elimination using cross-validation.

## **Parameters**

**\*\*kwargs** (*keyword arguments, optional*) – Additional options for esmvaltool. diag\_scripts.mlr. custom\_sklearn.cross\_val\_score\_weighted().

### export\_prediction\_data(filename=None)

Export all prediction data contained in *self.\_data*.

# Parameters

filename (str, optional (default: '{data\_type}\_{pred\_name}.csv')) Name of the exported files.

### export\_training\_data(filename=None)

Export all training data contained in *self.\_data*.

### **Parameters**

**filename** (*str*, *optional* (*default: '{data\_type}.csv'*)) – Name of the exported files.

# property features

Features of the input data.

Туре

numpy.ndarray

# property features\_after\_preprocessing

Features of the input data after preprocessing.

# Туре

numpy.ndarray

# property features\_types

Types of the features.

# Туре

pandas.Series

# property features\_units

Units of the features.

# Туре

pandas.Series

### fit()

Fit MLR model.

**Note:** Specifying keyword arguments for this function is not allowed here since *features\_after\_preprocessing* might be altered by that. Use the keyword argument fit\_kwargs during class initialization instead.

# property fit\_kwargs

Keyword arguments for fit().

Туре

dict

get\_ancestors(label=True, features=None, prediction\_names=None, prediction\_reference=False)
Return ancestor files.

#### **Parameters**

- label (bool, optional (default: True)) Return label files.
- **features** (*list of str*, *optional* (*default: None*)) Features for which files should be returned. If None, return files for all features.
- **prediction\_names** (list of str, optional (default: None)) Prediction names for which files should be returned. If None, return files for all prediction names.
- **prediction\_reference** (bool, optional (default: False)) Return prediction\_reference files if available for given prediction\_names.

#### Returns

Ancestor files.

# **Return type**

list of str

# Raises

**ValueError** – Invalid feature or prediction\_name given.

# get\_data\_frame(data\_type, impute\_nans=False)

Return data frame of specified type.

### Parameters

- **data\_type** (*str*) Data type to be returned. Must be one of 'all', 'train' or 'test'.
- impute\_nans (bool, optional (default: False)) Impute nans if desired.

#### Returns

Desired data.

# **Return type**

pandas.DataFrame

# Raises

**TypeError** – data\_type is invalid or data does not exist (e.g. test data is not set).

# get\_x\_array(data\_type, impute\_nans=False)

Return x data of specific type.

# Parameters

• **data\_type** (*str*) – Data type to be returned. Must be one of 'all', 'train' or 'test'.

• impute\_nans (bool, optional (default: False)) – Impute nans if desired.

### Returns

Desired data.

# Return type

numpy.ndarray

# Raises

**TypeError** – data\_type is invalid or data does not exist (e.g. test data is not set).

# get\_y\_array(data\_type, impute\_nans=False)

Return y data of specific type.

# Parameters

- **data\_type** (*str*) Data type to be returned. Must be one of 'all', 'train' or 'test'.
- impute\_nans (bool, optional (default: False)) Impute nans if desired.

### Returns

Desired data.

# **Return type**

numpy.ndarray

#### Raises

TypeError – data\_type is invalid or data does not exist (e.g. test data is not set).

# grid\_search\_cv(param\_grid, \*\*kwargs)

Perform exhaustive parameter search using cross-validation.

# Parameters

- **param\_grid** (*dict or list of dict*) Parameter names (keys) and ranges (values) for the search. Have to be given for each step of the pipeline separated by two underscores, i.e. s\_\_p is the parameter p for step s.
- **\*\*kwargs** (*keyword arguments, optional*) Additional options for sklearn. model\_selection.GridSearchCV.

# Raises

**ValueError** – Final regressor does not supply the attributes best\_estimator\_ or best\_params\_.

# property group\_attributes

Group attributes of the input data.

# Туре

numpy.ndarray

# property label

Label of the input data.

Type str

property label\_units

Units of the label.

#### Туре

str

### property mlr\_model\_type

MLR model type.

Туре

str

# property numerical\_features

Numerical features.

Type

# numpy.ndarray

# property parameters

Parameters of the complete MLR model pipeline.

# Туре

dict

# plot\_1d\_model(filename=None, n\_points=1000)

Plot lineplot that represents the MLR model.

Note: This only works for a model with a single feature.

# **Parameters**

- **filename** (*str*, *optional* (*default: '1d\_mlr\_model'*)) Name of the plot file.
- **n\_points** (*int*, *optional* (*default:* 1000)) Number of sampled points for the single feature (using linear spacing between minimum and maximum value).

# Raises

- sklearn.exceptions.NotFittedError MLR model is not fitted.
- ValueError MLR model is built from more than 1 feature.

# plot\_partial\_dependences(filename=None)

Plot partial dependences for every feature.

### Parameters

```
filename (str, optional (default: 'partial_dependece_{feature}')) -
Name of the plot file.
```

# Raises

sklearn.exceptions.NotFittedError – MLR model is not fitted.

# plot\_prediction\_errors(filename=None)

Plot predicted vs. true values.

# Parameters

**filename** (*str*, *optional* (*default: 'prediction\_errors'*)) – Name of the plot file.

### Raises

sklearn.exceptions.NotFittedError - MLR model is not fitted.

### plot\_residuals(filename=None)

Plot residuals of training and test (if available) data.

### Parameters

**filename** (*str*, *optional* (*default:* '*residuals*')) – Name of the plot file.

#### Raises

sklearn.exceptions.NotFittedError – MLR model is not fitted.

### plot\_residuals\_distribution(filename=None)

Plot distribution of residuals of training and test data (KDE).

# **Parameters**

**filename** (*str*, *optional* (*default:* '*residuals\_distribution*')) – Name of the plot file.

### Raises

sklearn.exceptions.NotFittedError – MLR model is not fitted.

#### plot\_residuals\_histogram(filename=None)

Plot histogram of residuals of training and test data.

# Parameters

**filename** (*str*, *optional* (*default:* '*residuals\_histogram*')) - Name of the plot file.

#### Raises

sklearn.exceptions.NotFittedError – MLR model is not fitted.

### plot\_scatterplots(filename=None)

Plot scatterplots label vs. feature for every feature.

### Parameters

filename (str, optional (default: 'scatterplot\_{feature}')) - Name of
the plot file.

#### Raises

sklearn.exceptions.NotFittedError - MLR model is not fitted.

# 

Perform prediction using the MLR model(s) and write \*.nc files.

#### **Parameters**

save\_mlr\_model\_error (str or int, optional) – Additionally saves estimated squared MLR model error. This error represents the uncertainty of the prediction caused by the MLR model itself and not by errors in the prediction input data (errors in that will be considered by including datasets with var\_type set to prediction\_input\_error and setting save\_propagated\_errors to True). If the option is set to 'test', the (constant) error is estimated as RMSEP using a (hold-out) test data set. Only possible if test data is available, i.e. the option test\_size is not set to False during class initialization. If the option is set to 'logo', the (constant) error is estimated as RMSEP using the group\_attributes. Only possible if group\_datasets\_by\_attributes is given. If the option is set to an integer n (!= 0), the (constant) error is estimated as RMSEP using n-fold cross-validation.

- **save\_lime\_importance** (*bool*, *optional* (*default: False*)) Additionally saves local feature importance given by LIME (Local Interpretable Model-agnostic Explanations).
- **save\_propagated\_errors** (*bool*, *optional* (*default: False*)) Additionally saves propagated errors from prediction\_input\_error datasets. Only possible when these are available.
- **\*\*kwargs** (*keyword arguments*, *optional*) Additional options for the final regressors predict() function.

# Raises

- RuntimeError return\_var and return\_cov are both set to True.
- sklearn.exceptions.NotFittedError MLR model is not fitted.
- ValueError An invalid value for save\_mlr\_model\_error is given.
- **ValueError** save\_propagated\_errors is True and no prediction\_input\_error data is available.

#### print\_correlation\_matrices()

Print correlation matrices for all datasets.

### print\_regression\_metrics(logo=False)

Print all available regression metrics for training data.

### **Parameters**

**logo** (bool, optional (default: False)) – Print regression metrics using sklearn.model\_selection.LeaveOneGroupOut cross-validation. Only possible when group\_datasets\_by\_attributes was given during class initialization.

# property random\_state

Random state instance.

Туре

numpy.random.RandomState

# classmethod register\_mlr\_model(mlr\_model\_type)

Add MLR model (subclass of this class) (decorator).

#### reset\_pipeline()

Reset regressor pipeline.

# rfecv(\*\*kwargs)

Perform recursive feature elimination using cross-validation.

**Note:** This only works for final estimators that provide information about feature importance either through a coef\_ attribute or through a feature\_importances\_ attribute.

#### **Parameters**

```
**kwargs (keyword arguments, optional) – Additional options for sklearn. feature_selection.RFECV.
```

### Raises

**RuntimeError** – Final estimator does not provide coef\_ or feature\_importances\_ attribute.

# test\_normality\_of\_residuals()

Perform Shapiro-Wilk test to normality of residuals.

# Raises

sklearn.exceptions.NotFittedError – MLR model is not fitted.

# update\_parameters(\*\*params)

Update parameters of the whole pipeline.

**Note:** Parameter names have to be given for each step of the pipeline separated by two underscores, i.e. s\_\_p is the parameter p for step s.

#### **Parameters**

**\*\*params** (keyword arguments, optional) – Parameters for the pipeline which should be updated.

### Raises

**ValueError** – Invalid parameter for pipeline given.

# LASSO Regression

Lasso Regression model.

Use mlr\_model\_type: lasso to use this MLR model in the recipe.

# Classes:

LassoModel(input\_datasets, \*\*kwargs) Lasso Regression model.

# class esmvaltool.diag\_scripts.mlr.models.lasso.LassoModel(input\_datasets, \*\*kwargs)

Bases: LinearModel

Lasso Regression model.

# Attributes:

categorical_features	Categorical features.
data	Input data of the MLR model.
features	Features of the input data.
features_after_preprocessing	Features of the input data after preprocessing.
features_types	Types of the features.
features_units	Units of the features.
fit_kwargs	Keyword arguments for <i>fit(</i> ).
group_attributes	Group attributes of the input data.
label	Label of the input data.
label_units	Units of the label.
mlr_model_type	MLR model type.
numerical_features	Numerical features.
parameters	Parameters of the complete MLR model pipeline.
random_state	Random state instance.

# Methods:

<pre>create(mlr_model_type, *args, **kwargs)</pre>	Create desired MLR model subclass (factory method).
efecv(**kwargs)	Perform exhaustive feature elimination using cross-validation.
<pre>export_prediction_data([filename])</pre>	Export all prediction data contained in <i>selfdata</i> .
<pre>export_training_data([filename])</pre>	Export all training data contained in <i>selfdata</i> .
fit()	Fit MLR model.
<pre>get_ancestors([label, features,])</pre>	Return ancestor files.
<pre>get_data_frame(data_type[, impute_nans])</pre>	Return data frame of specified type.
<pre>get_x_array(data_type[, impute_nans])</pre>	Return x data of specific type.
<pre>get_y_array(data_type[, impute_nans])</pre>	Return y data of specific type.
<pre>grid_search_cv(param_grid, **kwargs)</pre>	Perform exhaustive parameter search using cross-validation.
<pre>plot_1d_model([filename, n_points])</pre>	Plot lineplot that represents the MLR model.
<pre>plot_coefs([filename])</pre>	Plot linear coefficients of models.
<pre>plot_feature_importance([filename,</pre>	Plot feature importance given by linear coefficients.
color_coded])	
<pre>plot_partial_dependences([filename])</pre>	Plot partial dependences for every feature.
<pre>plot_prediction_errors([filename])</pre>	Plot predicted vs.
<pre>plot_residuals([filename])</pre>	Plot residuals of training and test (if available) data.
<pre>plot_residuals_distribution([filename])</pre>	Plot distribution of residuals of training and test data (KDE).
<pre>plot_residuals_histogram([filename])</pre>	Plot histogram of residuals of training and test data.
<pre>plot_scatterplots([filename])</pre>	Plot scatterplots label vs.
<pre>predict([save_mlr_model_error,])</pre>	Perform prediction using the MLR model(s) and write *.nc files.
<pre>print_correlation_matrices()</pre>	Print correlation matrices for all datasets.
<pre>print_regression_metrics([logo])</pre>	Print all available regression metrics for training data.
<pre>register_mlr_model(mlr_model_type)</pre>	Add MLR model (subclass of this class) (decorator).
reset_pipeline()	Reset regressor pipeline.
rfecv(**kwargs)	Perform recursive feature elimination using cross-validation.
<pre>test_normality_of_residuals()</pre>	Perform Shapiro-Wilk test to normality of residuals.
<pre>update_parameters(**params)</pre>	Update parameters of the whole pipeline.

# property categorical\_features

Categorical features.

# Туре

numpy.ndarray

classmethod create(mlr\_model\_type, \*args, \*\*kwargs)

Create desired MLR model subclass (factory method).

# property data

Input data of the MLR model.

Type dict

# efecv(\*\*kwargs)

Perform exhaustive feature elimination using cross-validation.

**\*\*kwargs** (*keyword arguments, optional*) – Additional options for esmvaltool. diag\_scripts.mlr. custom\_sklearn.cross\_val\_score\_weighted().

#### export\_prediction\_data(filename=None)

Export all prediction data contained in *self.\_data*.

### **Parameters**

```
filename (str, optional (default: '{data_type}_{pred_name}.csv')) -
Name of the exported files.
```

#### export\_training\_data(filename=None)

Export all training data contained in *self.\_data*.

### **Parameters**

```
filename (str, optional (default: '{data_type}.csv')) - Name of the exported files.
```

### property features

Features of the input data.

#### Туре

numpy.ndarray

### property features\_after\_preprocessing

Features of the input data after preprocessing.

### Туре

numpy.ndarray

#### property features\_types

Types of the features.

#### Туре

pandas.Series

# property features\_units

Units of the features.

# Туре

pandas.Series

#### fit()

Fit MLR model.

**Note:** Specifying keyword arguments for this function is not allowed here since *features\_after\_preprocessing* might be altered by that. Use the keyword argument *fit\_kwargs* during class initialization instead.

# property fit\_kwargs

Keyword arguments for fit().

Туре

dict

get\_ancestors(label=True, features=None, prediction\_names=None, prediction\_reference=False)
Return ancestor files.

- label (bool, optional (default: True)) Return label files.
- **features** (*list of str*, *optional* (*default: None*)) Features for which files should be returned. If None, return files for all features.
- **prediction\_names** (*list of str, optional (default: None*)) Prediction names for which files should be returned. If None, return files for all prediction names.
- **prediction\_reference** (bool, optional (default: False)) Return prediction\_reference files if available for given prediction\_names.

# Returns

Ancestor files.

#### **Return type**

list of str

# Raises

ValueError – Invalid feature or prediction\_name given.

# get\_data\_frame(data\_type, impute\_nans=False)

Return data frame of specified type.

# **Parameters**

- **data\_type** (*str*) Data type to be returned. Must be one of 'all', 'train' or 'test'.
- impute\_nans (bool, optional (default: False)) Impute nans if desired.

# Returns

Desired data.

### **Return type**

pandas.DataFrame

# Raises

**TypeError** – data\_type is invalid or data does not exist (e.g. test data is not set).

#### get\_x\_array(data\_type, impute\_nans=False)

Return x data of specific type.

#### Parameters

- **data\_type** (*str*) Data type to be returned. Must be one of 'all', 'train' or 'test'.
- impute\_nans (bool, optional (default: False)) Impute nans if desired.

#### Returns

Desired data.

# **Return type**

numpy.ndarray

# Raises

**TypeError** – data\_type is invalid or data does not exist (e.g. test data is not set).

#### get\_y\_array(data\_type, impute\_nans=False)

Return y data of specific type.

- **data\_type** (*str*) Data type to be returned. Must be one of 'all', 'train' or 'test'.
- impute\_nans (bool, optional (default: False)) Impute nans if desired.

# Returns

Desired data.

# **Return type**

numpy.ndarray

# Raises

TypeError – data\_type is invalid or data does not exist (e.g. test data is not set).

#### grid\_search\_cv(param\_grid, \*\*kwargs)

Perform exhaustive parameter search using cross-validation.

## **Parameters**

- **param\_grid** (*dict or list of dict*) Parameter names (keys) and ranges (values) for the search. Have to be given for each step of the pipeline separated by two underscores, i.e. s\_\_p is the parameter p for step s.
- **\*\*kwargs** (*keyword arguments, optional*) Additional options for sklearn. model\_selection.GridSearchCV.

#### Raises

**ValueError** – Final regressor does not supply the attributes best\_estimator\_ or best\_params\_.

# property group\_attributes

Group attributes of the input data.

# Туре

numpy.ndarray

property label

Label of the input data.

Type str

property label\_units

Units of the label.

# Туре

str

# property mlr\_model\_type

MLR model type.

# Туре

str

# property numerical\_features

Numerical features.

# Туре

numpy.ndarray

#### property parameters

Parameters of the complete MLR model pipeline.

Туре

# dict

```
plot_1d_model(filename=None, n_points=1000)
```

Plot lineplot that represents the MLR model.

Note: This only works for a model with a single feature.

### **Parameters**

- **filename** (str, optional (default: '1d\_mlr\_model')) Name of the plot file.
- **n\_points** (*int*, *optional* (*default:* 1000)) Number of sampled points for the single feature (using linear spacing between minimum and maximum value).

#### Raises

- sklearn.exceptions.NotFittedError MLR model is not fitted.
- ValueError MLR model is built from more than 1 feature.

### plot\_coefs(filename=None)

Plot linear coefficients of models.

Note: The features plotted here are not necessarily the real input features, but the ones after preprocessing.

# Parameters

filename (str, optional (default: 'coefs')) – Name of the plot file.

plot\_feature\_importance(filename=None, color\_coded=True)

Plot feature importance given by linear coefficients.

Note: The features plotted here are not necessarily the real input features, but the ones after preprocessing.

### Parameters

- filename (str, optional (default: 'feature\_importance')) Name of the plot file.
- **color\_coded** (*bool*, *optional* (*default: True*)) If True, mark positive (linear) correlations with red bars and negative (linear) correlations with blue bars. If False, all bars are blue.

### plot\_partial\_dependences(filename=None)

Plot partial dependences for every feature.

```
filename (str, optional (default: 'partial_dependece_{feature}')) -
Name of the plot file.
```

#### Raises

sklearn.exceptions.NotFittedError – MLR model is not fitted.

### plot\_prediction\_errors(filename=None)

Plot predicted vs. true values.

# Parameters

**filename**(*str*, *optional* (*default: 'prediction\_errors'*)) – Name of the plot file.

Raises

**sklearn.exceptions.NotFittedError** – MLR model is not fitted.

# plot\_residuals(filename=None)

Plot residuals of training and test (if available) data.

# Parameters

**filename** (*str*, *optional* (*default*: '*residuals*')) – Name of the plot file.

#### Raises

sklearn.exceptions.NotFittedError – MLR model is not fitted.

### plot\_residuals\_distribution(filename=None)

Plot distribution of residuals of training and test data (KDE).

#### **Parameters**

**filename** (*str*, *optional* (*default:* '*residuals\_distribution*')) – Name of the plot file.

#### Raises

sklearn.exceptions.NotFittedError - MLR model is not fitted.

## plot\_residuals\_histogram(filename=None)

Plot histogram of residuals of training and test data.

#### Parameters

**filename** (*str*, *optional* (*default: 'residuals\_histogram'*)) – Name of the plot file.

#### Raises

sklearn.exceptions.NotFittedError - MLR model is not fitted.

#### plot\_scatterplots(filename=None)

Plot scatterplots label vs. feature for every feature.

#### Parameters

filename (str, optional (default: 'scatterplot\_{feature}')) - Name of
the plot file.

Raises

sklearn.exceptions.NotFittedError – MLR model is not fitted.

# 

Perform prediction using the MLR model(s) and write \*.nc files.

#### **Parameters**

• **save\_mlr\_model\_error** (*str or int, optional*) – Additionally saves estimated squared MLR model error. This error represents the uncertainty of the prediction caused by the MLR model itself and not by errors in the prediction input data (errors in that will be considered by including datasets with var\_type set to prediction\_input\_error and setting save\_propagated\_errors to True). If the option is set to 'test', the (constant) error is estimated as RMSEP using a (hold-out) test data set. Only possible if test data is available, i.e. the option test\_size is not set to False during class initialization. If the option is set to 'logo', the (constant) error is estimated as RMSEP using leave-one-group-out cross-validation using the group\_attributes. Only possible if group\_datasets\_by\_attributes is given. If the option is set to an integer n (!= 0), the (constant) error is estimated as RMSEP using n-fold cross-validation.

- **save\_lime\_importance** (*bool*, *optional* (*default: False*)) Additionally saves local feature importance given by LIME (Local Interpretable Model-agnostic Explanations).
- **save\_propagated\_errors** (*bool*, *optional* (*default: False*)) Additionally saves propagated errors from prediction\_input\_error datasets. Only possible when these are available.
- **\*\*kwargs** (*keyword arguments*, *optional*) Additional options for the final regressors predict() function.

### Raises

- RuntimeError return\_var and return\_cov are both set to True.
- sklearn.exceptions.NotFittedError MLR model is not fitted.
- ValueError An invalid value for save\_mlr\_model\_error is given.
- **ValueError** save\_propagated\_errors is True and no prediction\_input\_error data is available.

### print\_correlation\_matrices()

Print correlation matrices for all datasets.

# print\_regression\_metrics(logo=False)

Print all available regression metrics for training data.

# **Parameters**

**logo** (bool, optional (default: False)) – Print regression metrics using sklearn.model\_selection.LeaveOneGroupOut cross-validation. Only possible when group\_datasets\_by\_attributes was given during class initialization.

# property random\_state

Random state instance.

# Туре

numpy.random.RandomState

# classmethod register\_mlr\_model(mlr\_model\_type)

Add MLR model (subclass of this class) (decorator).

# reset\_pipeline()

Reset regressor pipeline.

# rfecv(\*\*kwargs)

Perform recursive feature elimination using cross-validation.

**Note:** This only works for final estimators that provide information about feature importance either through a coef\_ attribute or through a feature\_importances\_ attribute.

# **Parameters**

```
**kwargs (keyword arguments, optional) - Additional options for sklearn. feature_selection.RFECV.
```

### Raises

**RuntimeError** – Final estimator does not provide coef\_ or feature\_importances\_ attribute.

# test\_normality\_of\_residuals()

Perform Shapiro-Wilk test to normality of residuals.

### Raises

sklearn.exceptions.NotFittedError – MLR model is not fitted.

# update\_parameters(\*\*params)

Update parameters of the whole pipeline.

**Note:** Parameter names have to be given for each step of the pipeline separated by two underscores, i.e. s\_\_p is the parameter p for step s.

#### **Parameters**

**\*\*params** (keyword arguments, optional) – Parameters for the pipeline which should be updated.

#### Raises

**ValueError** – Invalid parameter for pipeline given.

# LASSO Regression with built-in CV

Lasso Regression model with built-in CV.

Use mlr\_model\_type: lasso\_cv to use this MLR model in the recipe.

# **Classes:**

Lasso Regression model with built-in CV.

class esmvaltool.diag\_scripts.mlr.models.lasso\_cv.LassoCVModel(input\_datasets, \*\*kwargs)
Bases: LinearModel

Lasso Regression model with built-in CV.

Attributes:

categorical_features	Categorical features.
data	Input data of the MLR model.
features	Features of the input data.
features_after_preprocessing	Features of the input data after preprocessing.
features_types	Types of the features.
features_units	Units of the features.
fit_kwargs	Keyword arguments for fit().
group_attributes	Group attributes of the input data.
label	Label of the input data.
label_units	Units of the label.
mlr_model_type	MLR model type.
numerical_features	Numerical features.
parameters	Parameters of the complete MLR model pipeline.
random_state	Random state instance.

# Methods:

<pre>create(mlr_model_type, *args, **kwargs)</pre>	Create desired MLR model subclass (factory method).
efecv(**kwargs)	Perform exhaustive feature elimination using cross-validation.
<pre>export_prediction_data([filename])</pre>	Export all prediction data contained in <i>selfdata</i> .
<pre>export_training_data([filename])</pre>	Export all training data contained in <i>selfdata</i> .
<pre>fit()</pre>	Print final alpha after successful fitting.
<pre>get_ancestors([label, features,])</pre>	Return ancestor files.
<pre>get_data_frame(data_type[, impute_nans])</pre>	Return data frame of specified type.
<pre>get_x_array(data_type[, impute_nans])</pre>	Return x data of specific type.
<pre>get_y_array(data_type[, impute_nans])</pre>	Return y data of specific type.
<pre>grid_search_cv(param_grid, **kwargs)</pre>	Perform exhaustive parameter search using cross-validation.
<pre>plot_1d_model([filename, n_points])</pre>	Plot lineplot that represents the MLR model.
<pre>plot_coefs([filename])</pre>	Plot linear coefficients of models.
<pre>plot_feature_importance([filename,</pre>	Plot feature importance given by linear coefficients.
color_coded])	
<pre>plot_partial_dependences([filename])</pre>	Plot partial dependences for every feature.
<pre>plot_prediction_errors([filename])</pre>	Plot predicted vs.
<pre>plot_residuals([filename])</pre>	Plot residuals of training and test (if available) data.
<pre>plot_residuals_distribution([filename])</pre>	Plot distribution of residuals of training and test data (KDE).
<pre>plot_residuals_histogram([filename])</pre>	Plot histogram of residuals of training and test data.
<pre>plot_scatterplots([filename])</pre>	Plot scatterplots label vs.
<pre>predict([save_mlr_model_error,])</pre>	Perform prediction using the MLR model(s) and write *.nc files.
<pre>print_correlation_matrices()</pre>	Print correlation matrices for all datasets.
<pre>print_regression_metrics([logo])</pre>	Print all available regression metrics for training data.
<pre>register_mlr_model(mlr_model_type)</pre>	Add MLR model (subclass of this class) (decorator).
reset_pipeline()	Reset regressor pipeline.
rfecv(**kwargs)	Perform recursive feature elimination using cross-validation.
<pre>test_normality_of_residuals()</pre>	Perform Shapiro-Wilk test to normality of residuals.
update_parameters(**params)	Update parameters of the whole pipeline.

# property categorical\_features

Categorical features.

Туре

numpy.ndarray

```
classmethod create(mlr_model_type, *args, **kwargs)
```

Create desired MLR model subclass (factory method).

# property data

Input data of the MLR model.

Туре

dict

# efecv(\*\*kwargs)

Perform exhaustive feature elimination using cross-validation.

# Parameters

```
**kwargs (keyword arguments, optional) – Additional options for esmvaltool. diag_scripts.mlr. custom_sklearn.cross_val_score_weighted().
```

### export\_prediction\_data(filename=None)

Export all prediction data contained in *self.\_data*.

# Parameters

```
filename (str, optional (default: '{data_type}_{pred_name}.csv')) -
Name of the exported files.
```

# export\_training\_data(filename=None)

Export all training data contained in *self.\_data*.

#### Parameters

```
filename (str, optional (default: '{data_type}.csv')) - Name of the exported files.
```

# property features

Features of the input data.

Туре

numpy.ndarray

# property features\_after\_preprocessing

Features of the input data after preprocessing.

### Type

numpy.ndarray

# property features\_types

Types of the features.

Туре

pandas.Series

property features\_units

Units of the features.

Туре

pandas.Series

# fit()

Print final alpha after successful fitting.

# property fit\_kwargs

Keyword arguments for *fit(*).

# Туре

dict

get\_ancestors(label=True, features=None, prediction\_names=None, prediction\_reference=False)
Return ancestor files.

# Parameters

- label (bool, optional (default: True)) Return label files.
- **features** (*list of str*, *optional* (*default: None*)) Features for which files should be returned. If None, return files for all features.
- prediction\_names (list of str, optional (default: None)) Prediction names for which files should be returned. If None, return files for all prediction names.
- **prediction\_reference** (bool, optional (default: False)) Return prediction\_reference files if available for given prediction\_names.

#### Returns

Ancestor files.

Return type

list of str

# Raises

**ValueError** – Invalid feature or prediction\_name given.

## get\_data\_frame(data\_type, impute\_nans=False)

Return data frame of specified type.

# Parameters

- **data\_type** (*str*) Data type to be returned. Must be one of 'all', 'train' or 'test'.
- impute\_nans (bool, optional (default: False)) Impute nans if desired.

### Returns

Desired data.

# **Return type**

pandas.DataFrame

# Raises

**TypeError** – data\_type is invalid or data does not exist (e.g. test data is not set).

### get\_x\_array(data\_type, impute\_nans=False)

Return x data of specific type.

- **data\_type** (*str*) Data type to be returned. Must be one of 'all', 'train' or 'test'.
- impute\_nans (bool, optional (default: False)) Impute nans if desired.

### Returns

Desired data.

# **Return type**

numpy.ndarray

# Raises

**TypeError** – data\_type is invalid or data does not exist (e.g. test data is not set).

#### get\_y\_array(data\_type, impute\_nans=False)

Return y data of specific type.

# Parameters

- **data\_type** (*str*) Data type to be returned. Must be one of 'all', 'train' or 'test'.
- impute\_nans (bool, optional (default: False)) Impute nans if desired.

### Returns

Desired data.

# Return type

numpy.ndarray

#### Raises

**TypeError** – data\_type is invalid or data does not exist (e.g. test data is not set).

# grid\_search\_cv(param\_grid, \*\*kwargs)

Perform exhaustive parameter search using cross-validation.

### **Parameters**

- **param\_grid** (*dict or list of dict*) Parameter names (keys) and ranges (values) for the search. Have to be given for each step of the pipeline separated by two underscores, i.e. s\_\_p is the parameter p for step s.
- **\*\*kwargs** (*keyword arguments, optional*) Additional options for sklearn. model\_selection.GridSearchCV.

# Raises

**ValueError** – Final regressor does not supply the attributes best\_estimator\_ or best\_params\_.

# property group\_attributes

Group attributes of the input data.

### Туре

numpy.ndarray

# property label

Label of the input data.

Type str

property label\_units

Units of the label.

Туре

str

### property mlr\_model\_type

MLR model type.

Туре

str

# property numerical\_features

Numerical features.

Type

# numpy.ndarray

# property parameters

Parameters of the complete MLR model pipeline.

# Туре

dict

# plot\_1d\_model(filename=None, n\_points=1000)

Plot lineplot that represents the MLR model.

Note: This only works for a model with a single feature.

# **Parameters**

- **filename** (*str*, *optional* (*default: '1d\_mlr\_model'*)) Name of the plot file.
- **n\_points** (*int*, *optional* (*default:* 1000)) Number of sampled points for the single feature (using linear spacing between minimum and maximum value).

# Raises

- sklearn.exceptions.NotFittedError MLR model is not fitted.
- ValueError MLR model is built from more than 1 feature.

# plot\_coefs(filename=None)

Plot linear coefficients of models.

Note: The features plotted here are not necessarily the real input features, but the ones after preprocessing.

# Parameters

filename (str, optional (default: 'coefs')) – Name of the plot file.

plot\_feature\_importance(filename=None, color\_coded=True)

Plot feature importance given by linear coefficients.

Note: The features plotted here are not necessarily the real input features, but the ones after preprocessing.

# **Parameters**

• filename (str, optional (default: 'feature\_importance')) - Name of the plot file.

• **color\_coded** (*bool*, *optional* (*default: True*)) – If True, mark positive (linear) correlations with red bars and negative (linear) correlations with blue bars. If False, all bars are blue.

plot\_partial\_dependences(filename=None)

Plot partial dependences for every feature.

# Parameters

```
filename (str, optional (default: 'partial_dependece_{feature}')) - Name of the plot file.
```

Raises

sklearn.exceptions.NotFittedError - MLR model is not fitted.

### plot\_prediction\_errors(filename=None)

Plot predicted vs. true values.

# Parameters

**filename** (*str*, *optional* (*default:* '*prediction\_errors*')) – Name of the plot file.

Raises

sklearn.exceptions.NotFittedError – MLR model is not fitted.

### plot\_residuals(filename=None)

Plot residuals of training and test (if available) data.

### **Parameters**

**filename** (*str*, *optional* (*default:* '*residuals*')) – Name of the plot file.

#### Raises

sklearn.exceptions.NotFittedError – MLR model is not fitted.

# plot\_residuals\_distribution(filename=None)

Plot distribution of residuals of training and test data (KDE).

### Parameters

**filename** (*str*, *optional* (*default:* '*residuals\_distribution*')) – Name of the plot file.

#### Raises

sklearn.exceptions.NotFittedError – MLR model is not fitted.

### plot\_residuals\_histogram(filename=None)

Plot histogram of residuals of training and test data.

# Parameters

**filename** (*str*, *optional* (*default:* '*residuals\_histogram*')) – Name of the plot file.

# Raises

sklearn.exceptions.NotFittedError – MLR model is not fitted.

# plot\_scatterplots(filename=None)

Plot scatterplots label vs. feature for every feature.

# Parameters

filename (str, optional (default: 'scatterplot\_{feature}')) - Name of
the plot file.

### Raises

sklearn.exceptions.NotFittedError – MLR model is not fitted.

Perform prediction using the MLR model(s) and write \*.nc files.

### Parameters

- save\_mlr\_model\_error (str or int, optional) Additionally saves estimated squared MLR model error. This error represents the uncertainty of the prediction caused by the MLR model itself and not by errors in the prediction input data (errors in that will be considered by including datasets with var\_type set to prediction\_input\_error and setting save\_propagated\_errors to True). If the option is set to 'test', the (constant) error is estimated as RMSEP using a (hold-out) test data set. Only possible if test data is available, i.e. the option test\_size is not set to False during class initialization. If the option is set to 'logo', the (constant) error is estimated as RMSEP using the group\_attributes. Only possible if group\_datasets\_by\_attributes is given. If the option is set to an integer n (!= 0), the (constant) error is estimated as RMSEP using n-fold cross-validation.
- **save\_lime\_importance** (*bool*, *optional* (*default: False*)) Additionally saves local feature importance given by LIME (Local Interpretable Model-agnostic Explanations).
- **save\_propagated\_errors** (*bool*, *optional* (*default: False*)) Additionally saves propagated errors from prediction\_input\_error datasets. Only possible when these are available.
- **\*\*kwargs** (*keyword arguments*, *optional*) Additional options for the final regressors predict() function.

# Raises

- RuntimeError return\_var and return\_cov are both set to True.
- sklearn.exceptions.NotFittedError MLR model is not fitted.
- ValueError An invalid value for save\_mlr\_model\_error is given.
- **ValueError** save\_propagated\_errors is True and no prediction\_input\_error data is available.

#### print\_correlation\_matrices()

Print correlation matrices for all datasets.

# print\_regression\_metrics(logo=False)

Print all available regression metrics for training data.

### Parameters

**logo** (bool, optional (default: False)) – Print regression metrics using sklearn.model\_selection.LeaveOneGroupOut cross-validation. Only possible when group\_datasets\_by\_attributes was given during class initialization.

# property random\_state

Random state instance.

Туре

numpy.random.RandomState

### classmethod register\_mlr\_model(mlr\_model\_type)

Add MLR model (subclass of this class) (decorator).

### reset\_pipeline()

Reset regressor pipeline.

### rfecv(\*\*kwargs)

Perform recursive feature elimination using cross-validation.

**Note:** This only works for final estimators that provide information about feature importance either through a coef\_ attribute or through a feature\_importances\_ attribute.

### **Parameters**

```
**kwargs (keyword arguments, optional) - Additional options for sklearn. feature_selection.RFECV.
```

### Raises

**RuntimeError** – Final estimator does not provide coef\_ or feature\_importances\_ attribute.

### test\_normality\_of\_residuals()

Perform Shapiro-Wilk test to normality of residuals.

#### Raises

sklearn.exceptions.NotFittedError – MLR model is not fitted.

#### update\_parameters(\*\*params)

Update parameters of the whole pipeline.

**Note:** Parameter names have to be given for each step of the pipeline separated by two underscores, i.e. s\_\_p is the parameter p for step s.

#### **Parameters**

**\*\*params** (keyword arguments, optional) – Parameters for the pipeline which should be updated.

### Raises

**ValueError** – Invalid parameter for pipeline given.

### LASSO Regression (using Least-angle Regression algorithm) with built-in CV

Lasso Regression model with built-in CV using LARS algorithm.

Use mlr\_model\_type: lasso\_lars\_cv to use this MLR model in the recipe.

# Classes:

LassoLarsCVModel(input_datasets, **kwargs)	Lasso Regression model with built-in CV using LARS
	algorithm.

class esmvaltool.diag\_scripts.mlr.models.lasso\_lars\_cv.LassoLarsCVModel(input\_datasets,

\*\*kwargs)

# Bases: LinearModel

Lasso Regression model with built-in CV using LARS algorithm.

# Attributes:

categorical_features	Categorical features.
data	Input data of the MLR model.
features	Features of the input data.
features_after_preprocessing	Features of the input data after preprocessing.
features_types	Types of the features.
features_units	Units of the features.
fit_kwargs	Keyword arguments for <i>fit(</i> ).
group_attributes	Group attributes of the input data.
label	Label of the input data.
label_units	Units of the label.
mlr_model_type	MLR model type.
numerical_features	Numerical features.
parameters	Parameters of the complete MLR model pipeline.
random_state	Random state instance.

Methods:

<pre>create(mlr_model_type, *args, **kwargs)</pre>	Create desired MLR model subclass (factory method).
efecv(**kwargs)	Perform exhaustive feature elimination using cross-validation.
<pre>export_prediction_data([filename])</pre>	Export all prediction data contained in <i>selfdata</i> .
<pre>export_training_data([filename])</pre>	Export all training data contained in <i>selfdata</i> .
fit()	Print final alpha after successful fitting.
<pre>get_ancestors([label, features,])</pre>	Return ancestor files.
<pre>get_data_frame(data_type[, impute_nans])</pre>	Return data frame of specified type.
<pre>get_x_array(data_type[, impute_nans])</pre>	Return x data of specific type.
<pre>get_y_array(data_type[, impute_nans])</pre>	Return y data of specific type.
<pre>grid_search_cv(param_grid, **kwargs)</pre>	Perform exhaustive parameter search using cross-validation.
<pre>plot_1d_model([filename, n_points])</pre>	Plot lineplot that represents the MLR model.
<pre>plot_coefs([filename])</pre>	Plot linear coefficients of models.
<pre>plot_feature_importance([filename,</pre>	Plot feature importance given by linear coefficients.
color_coded])	
<pre>plot_partial_dependences([filename])</pre>	Plot partial dependences for every feature.
<pre>plot_prediction_errors([filename])</pre>	Plot predicted vs.
<pre>plot_residuals([filename])</pre>	Plot residuals of training and test (if available) data.
<pre>plot_residuals_distribution([filename])</pre>	Plot distribution of residuals of training and test data (KDE).
<pre>plot_residuals_histogram([filename])</pre>	Plot histogram of residuals of training and test data.
<pre>plot_scatterplots([filename])</pre>	Plot scatterplots label vs.
<pre>predict([save_mlr_model_error,])</pre>	Perform prediction using the MLR model(s) and write *.nc files.
<pre>print_correlation_matrices()</pre>	Print correlation matrices for all datasets.
<pre>print_regression_metrics([logo])</pre>	Print all available regression metrics for training data.
<pre>register_mlr_model(mlr_model_type)</pre>	Add MLR model (subclass of this class) (decorator).
reset_pipeline()	Reset regressor pipeline.
<pre>rfecv(**kwargs)</pre>	Perform recursive feature elimination using cross-validation.
<pre>test_normality_of_residuals()</pre>	Perform Shapiro-Wilk test to normality of residuals.
update_parameters(**params)	Update parameters of the whole pipeline.

# property categorical\_features

Categorical features.

# Туре

numpy.ndarray

classmethod create(mlr\_model\_type, \*args, \*\*kwargs)

Create desired MLR model subclass (factory method).

# property data

Input data of the MLR model.

Type dict

efecv(\*\*kwargs)

Perform exhaustive feature elimination using cross-validation.

**\*\*kwargs** (*keyword arguments, optional*) – Additional options for esmvaltool. diag\_scripts.mlr. custom\_sklearn.cross\_val\_score\_weighted().

#### export\_prediction\_data(filename=None)

Export all prediction data contained in *self.\_data*.

### **Parameters**

```
filename (str, optional (default: '{data_type}_{pred_name}.csv')) -
Name of the exported files.
```

### export\_training\_data(filename=None)

Export all training data contained in *self.\_data*.

### **Parameters**

```
filename (str, optional (default: '{data_type}.csv')) - Name of the exported files.
```

### property features

Features of the input data.

### Туре

numpy.ndarray

# property features\_after\_preprocessing

Features of the input data after preprocessing.

Туре

numpy.ndarray

# property features\_types

Types of the features.

#### Туре

pandas.Series

# property features\_units

Units of the features.

Туре

pandas.Series

# fit()

Print final alpha after successful fitting.

# property fit\_kwargs

Keyword arguments for fit().

# Туре

dict

get\_ancestors(label=True, features=None, prediction\_names=None, prediction\_reference=False)
Return ancestor files.

- label (bool, optional (default: True)) Return label files.
- **features** (*list of str*, *optional (default: None*)) Features for which files should be returned. If None, return files for all features.

- **prediction\_names** (list of str, optional (default: None)) Prediction names for which files should be returned. If None, return files for all prediction names.
- prediction\_reference (bool, optional (default: False)) Return prediction\_reference files if available for given prediction\_names.

# Returns

Ancestor files.

# **Return type**

list of str

# Raises

ValueError – Invalid feature or prediction\_name given.

### get\_data\_frame(data\_type, impute\_nans=False)

Return data frame of specified type.

# Parameters

- **data\_type** (*str*) Data type to be returned. Must be one of 'all', 'train' or 'test'.
- impute\_nans (bool, optional (default: False)) Impute nans if desired.

### Returns

Desired data.

# Return type

pandas.DataFrame

# Raises

**TypeError** – data\_type is invalid or data does not exist (e.g. test data is not set).

### get\_x\_array(data\_type, impute\_nans=False)

Return x data of specific type.

# Parameters

- **data\_type** (*str*) Data type to be returned. Must be one of 'all', 'train' or 'test'.
- impute\_nans (bool, optional (default: False)) Impute nans if desired.

# Returns

Desired data.

# Return type

numpy.ndarray

# Raises

**TypeError** – data\_type is invalid or data does not exist (e.g. test data is not set).

# get\_y\_array(data\_type, impute\_nans=False)

Return y data of specific type.

- **data\_type** (*str*) Data type to be returned. Must be one of 'all', 'train' or 'test'.
- **impute\_nans** (bool, optional (default: False)) Impute nans if desired.

# Returns

Desired data.

# **Return type**

numpy.ndarray

# Raises

**TypeError** – data\_type is invalid or data does not exist (e.g. test data is not set).

### grid\_search\_cv(param\_grid, \*\*kwargs)

Perform exhaustive parameter search using cross-validation.

### **Parameters**

- **param\_grid** (*dict or list of dict*) Parameter names (keys) and ranges (values) for the search. Have to be given for each step of the pipeline separated by two underscores, i.e. s\_\_p is the parameter p for step s.
- **\*\*kwargs** (*keyword arguments, optional*) Additional options for sklearn. model\_selection.GridSearchCV.

# Raises

**ValueError** – Final regressor does not supply the attributes best\_estimator\_ or best\_params\_.

# property group\_attributes

Group attributes of the input data.

Туре

numpy.ndarray

# property label

Label of the input data.

# Туре

str

property label\_units

Units of the label.

Type str

property mlr\_model\_type

MLR model type.

# Туре

str

# property numerical\_features

Numerical features.

# Туре

numpy.ndarray

# property parameters

Parameters of the complete MLR model pipeline.

Туре

dict

#### plot\_1d\_model(filename=None, n\_points=1000)

Plot lineplot that represents the MLR model.

Note: This only works for a model with a single feature.

# Parameters

- filename (str, optional (default: '1d\_mlr\_model')) Name of the plot file.
- **n\_points** (*int*, *optional* (*default:* 1000)) Number of sampled points for the single feature (using linear spacing between minimum and maximum value).

#### Raises

- sklearn.exceptions.NotFittedError MLR model is not fitted.
- ValueError MLR model is built from more than 1 feature.

### plot\_coefs(filename=None)

Plot linear coefficients of models.

Note: The features plotted here are not necessarily the real input features, but the ones after preprocessing.

#### **Parameters**

**filename** (*str*, *optional* (*default:* '*coefs*')) – Name of the plot file.

#### plot\_feature\_importance(filename=None, color\_coded=True)

Plot feature importance given by linear coefficients.

Note: The features plotted here are not necessarily the real input features, but the ones after preprocessing.

### **Parameters**

- **filename** (*str*, *optional* (*default:* '*feature\_importance*')) Name of the plot file.
- **color\_coded** (*bool*, *optional* (*default: True*)) If True, mark positive (linear) correlations with red bars and negative (linear) correlations with blue bars. If False, all bars are blue.

### plot\_partial\_dependences(filename=None)

Plot partial dependences for every feature.

#### Parameters

filename (str, optional (default: 'partial\_dependece\_{feature}')) Name of the plot file.

### Raises

sklearn.exceptions.NotFittedError – MLR model is not fitted.

#### plot\_prediction\_errors(filename=None)

Plot predicted vs. true values.

### Parameters

**filename** (*str*, *optional* (*default:* '*prediction\_errors*')) – Name of the plot file.

#### Raises

sklearn.exceptions.NotFittedError – MLR model is not fitted.

#### plot\_residuals(filename=None)

Plot residuals of training and test (if available) data.

### Parameters

**filename** (*str*, *optional* (*default:* '*residuals*')) – Name of the plot file.

#### Raises

sklearn.exceptions.NotFittedError - MLR model is not fitted.

### plot\_residuals\_distribution(filename=None)

Plot distribution of residuals of training and test data (KDE).

### Parameters

**filename** (*str*, *optional* (*default:* '*residuals\_distribution*')) – Name of the plot file.

#### Raises

sklearn.exceptions.NotFittedError – MLR model is not fitted.

#### plot\_residuals\_histogram(filename=None)

Plot histogram of residuals of training and test data.

#### Parameters

**filename** (*str*, *optional* (*default: 'residuals\_histogram'*)) – Name of the plot file.

Raises

sklearn.exceptions.NotFittedError – MLR model is not fitted.

## plot\_scatterplots(filename=None)

Plot scatterplots label vs. feature for every feature.

### Parameters

**filename** (*str*, *optional* (*default: 'scatterplot\_{feature}'*)) – Name of the plot file.

Raises

sklearn.exceptions.NotFittedError - MLR model is not fitted.

Perform prediction using the MLR model(s) and write \*.nc files.

#### Parameters

• **save\_mlr\_model\_error** (*str or int, optional*) – Additionally saves estimated squared MLR model error. This error represents the uncertainty of the prediction caused by the MLR model itself and not by errors in the prediction input data (errors in that will be considered by including datasets with var\_type set to prediction\_input\_error and setting save\_propagated\_errors to True). If the option is set to 'test', the (constant) error is estimated as RMSEP using a (hold-out)

test data set. Only possible if test data is available, i.e. the option test\_size is not set to False during class initialization. If the option is set to 'logo', the (constant) error is estimated as RMSEP using leave-one-group-out cross-validation using the group\_attributes. Only possible if group\_datasets\_by\_attributes is given. If the option is set to an integer n (!= 0), the (constant) error is estimated as RMSEP using n-fold cross-validation.

- **save\_lime\_importance** (*bool*, *optional* (*default: False*)) Additionally saves local feature importance given by LIME (Local Interpretable Model-agnostic Explanations).
- **save\_propagated\_errors** (*bool*, *optional* (*default: False*)) Additionally saves propagated errors from prediction\_input\_error datasets. Only possible when these are available.
- **\*\*kwargs** (*keyword arguments*, *optional*) Additional options for the final regressors predict() function.

### Raises

- RuntimeError return\_var and return\_cov are both set to True.
- sklearn.exceptions.NotFittedError MLR model is not fitted.
- ValueError An invalid value for save\_mlr\_model\_error is given.
- **ValueError** save\_propagated\_errors is True and no prediction\_input\_error data is available.

#### print\_correlation\_matrices()

Print correlation matrices for all datasets.

#### print\_regression\_metrics(logo=False)

Print all available regression metrics for training data.

#### Parameters

**logo** (bool, optional (default: False)) – Print regression metrics using sklearn.model\_selection.LeaveOneGroupOut cross-validation. Only possible when group\_datasets\_by\_attributes was given during class initialization.

#### property random\_state

Random state instance.

#### Type

numpy.random.RandomState

### classmethod register\_mlr\_model(mlr\_model\_type)

Add MLR model (subclass of this class) (decorator).

### reset\_pipeline()

Reset regressor pipeline.

### rfecv(\*\*kwargs)

Perform recursive feature elimination using cross-validation.

**Note:** This only works for final estimators that provide information about feature importance either through a coef\_ attribute or through a feature\_importances\_ attribute.

### **Parameters**

**\*\*kwargs** (*keyword arguments, optional*) – Additional options for sklearn. feature\_selection.RFECV.

### Raises

**RuntimeError** – Final estimator does not provide coef\_ or feature\_importances\_ attribute.

# test\_normality\_of\_residuals()

Perform Shapiro-Wilk test to normality of residuals.

### Raises

sklearn.exceptions.NotFittedError – MLR model is not fitted.

### update\_parameters(\*\*params)

Update parameters of the whole pipeline.

**Note:** Parameter names have to be given for each step of the pipeline separated by two underscores, i.e. s\_\_p is the parameter p for step s.

#### **Parameters**

**\*\*params** (keyword arguments, optional) – Parameters for the pipeline which should be updated.

# Raises

**ValueError** – Invalid parameter for pipeline given.

## **Linear Regression**

Linear Regression model.

Use mlr\_model\_type: linear to use this MLR model in the recipe.

### **Classes:**

LinearRegressionModel(input\_datasets, \*\*kwargs) Linear Regression model.

class esmvaltool.diag\_scripts.mlr.models.linear.LinearRegressionModel(input\_datasets,

\*\*kwargs)

Bases: LinearModel
Linear Regression model.

Attributes:

categorical_features	Categorical features.
data	Input data of the MLR model.
features	Features of the input data.
features_after_preprocessing	Features of the input data after preprocessing.
features_types	Types of the features.
features_units	Units of the features.
fit_kwargs	Keyword arguments for <i>fit(</i> ).
group_attributes	Group attributes of the input data.
label	Label of the input data.
label_units	Units of the label.
mlr_model_type	MLR model type.
numerical_features	Numerical features.
parameters	Parameters of the complete MLR model pipeline.
random_state	Random state instance.

# Methods:

<pre>create(mlr_model_type, *args, **kwargs)</pre>	Create desired MLR model subclass (factory method).
efecv(**kwargs)	Perform exhaustive feature elimination using cross-validation.
<pre>export_prediction_data([filename])</pre>	Export all prediction data contained in <i>selfdata</i> .
<pre>export_training_data([filename])</pre>	Export all training data contained in <i>selfdata</i> .
fit()	Fit MLR model.
<pre>get_ancestors([label, features,])</pre>	Return ancestor files.
<pre>get_data_frame(data_type[, impute_nans])</pre>	Return data frame of specified type.
<pre>get_x_array(data_type[, impute_nans])</pre>	Return x data of specific type.
<pre>get_y_array(data_type[, impute_nans])</pre>	Return y data of specific type.
<pre>grid_search_cv(param_grid, **kwargs)</pre>	Perform exhaustive parameter search using cross-validation.
<pre>plot_1d_model([filename, n_points])</pre>	Plot lineplot that represents the MLR model.
<pre>plot_coefs([filename])</pre>	Plot linear coefficients of models.
<pre>plot_feature_importance([filename,</pre>	Plot feature importance given by linear coefficients.
color_coded])	
<pre>plot_partial_dependences([filename])</pre>	Plot partial dependences for every feature.
<pre>plot_prediction_errors([filename])</pre>	Plot predicted vs.
<pre>plot_residuals([filename])</pre>	Plot residuals of training and test (if available) data.
<pre>plot_residuals_distribution([filename])</pre>	Plot distribution of residuals of training and test data (KDE).
<pre>plot_residuals_histogram([filename])</pre>	Plot histogram of residuals of training and test data.
<pre>plot_scatterplots([filename])</pre>	Plot scatterplots label vs.
<pre>predict([save_mlr_model_error,])</pre>	Perform prediction using the MLR model(s) and write *.nc files.
<pre>print_correlation_matrices()</pre>	Print correlation matrices for all datasets.
<pre>print_regression_metrics([logo])</pre>	Print all available regression metrics for training data.
<pre>register_mlr_model(mlr_model_type)</pre>	Add MLR model (subclass of this class) (decorator).
reset_pipeline()	Reset regressor pipeline.
rfecv(**kwargs)	Perform recursive feature elimination using cross-validation.
<pre>test_normality_of_residuals()</pre>	Perform Shapiro-Wilk test to normality of residuals.
update_parameters(**params)	Update parameters of the whole pipeline.

### property categorical\_features

Categorical features.

### Туре

numpy.ndarray

```
classmethod create(mlr_model_type, *args, **kwargs)
```

Create desired MLR model subclass (factory method).

# property data

Input data of the MLR model.

Туре

dict

# efecv(\*\*kwargs)

Perform exhaustive feature elimination using cross-validation.

## Parameters

```
**kwargs (keyword arguments, optional) – Additional options for esmvaltool. diag_scripts.mlr. custom_sklearn.cross_val_score_weighted().
```

### export\_prediction\_data(filename=None)

Export all prediction data contained in *self.\_data*.

### Parameters

```
filename (str, optional (default: '{data_type}_{pred_name}.csv')) -
Name of the exported files.
```

# export\_training\_data(filename=None)

Export all training data contained in *self.\_data*.

#### **Parameters**

```
filename (str, optional (default: '{data_type}.csv')) - Name of the exported files.
```

# property features

Features of the input data.

# Туре

numpy.ndarray

## property features\_after\_preprocessing

Features of the input data after preprocessing.

### Туре

numpy.ndarray

# property features\_types

Types of the features.

Туре

pandas.Series

# property features\_units

Units of the features.

### Туре

pandas.Series

### fit()

Fit MLR model.

**Note:** Specifying keyword arguments for this function is not allowed here since *features\_after\_preprocessing* might be altered by that. Use the keyword argument fit\_kwargs during class initialization instead.

## property fit\_kwargs

Keyword arguments for *fit(*).

# Туре

dict

get\_ancestors(label=True, features=None, prediction\_names=None, prediction\_reference=False)
Return ancestor files.

#### **Parameters**

- label (bool, optional (default: True)) Return label files.
- **features** (*list of str*, *optional* (*default: None*)) Features for which files should be returned. If None, return files for all features.
- **prediction\_names** (list of str, optional (default: None)) Prediction names for which files should be returned. If None, return files for all prediction names.
- **prediction\_reference** (bool, optional (default: False)) Return prediction\_reference files if available for given prediction\_names.

#### Returns

Ancestor files.

# **Return type**

list of str

## Raises

ValueError – Invalid feature or prediction\_name given.

# get\_data\_frame(data\_type, impute\_nans=False)

Return data frame of specified type.

#### **Parameters**

- **data\_type** (*str*) Data type to be returned. Must be one of 'all', 'train' or 'test'.
- impute\_nans (bool, optional (default: False)) Impute nans if desired.

#### Returns

Desired data.

### **Return type**

pandas.DataFrame

# Raises

**TypeError** – data\_type is invalid or data does not exist (e.g. test data is not set).

### get\_x\_array(data\_type, impute\_nans=False)

Return x data of specific type.

## Parameters

- **data\_type** (*str*) Data type to be returned. Must be one of 'all', 'train' or 'test'.
- impute\_nans (bool, optional (default: False)) Impute nans if desired.

#### Returns

Desired data.

# **Return type**

numpy.ndarray

### Raises

**TypeError** – data\_type is invalid or data does not exist (e.g. test data is not set).

#### get\_y\_array(data\_type, impute\_nans=False)

Return y data of specific type.

#### **Parameters**

- **data\_type** (*str*) Data type to be returned. Must be one of 'all', 'train' or 'test'.
- impute\_nans (bool, optional (default: False)) Impute nans if desired.

#### Returns

Desired data.

### Return type numpy.ndarray

#### Raises

**TypeError** – data\_type is invalid or data does not exist (e.g. test data is not set).

### grid\_search\_cv(param\_grid, \*\*kwargs)

Perform exhaustive parameter search using cross-validation.

### **Parameters**

- **param\_grid** (*dict or list of dict*) Parameter names (keys) and ranges (values) for the search. Have to be given for each step of the pipeline separated by two underscores, i.e. s\_\_p is the parameter p for step s.
- **\*\*kwargs** (*keyword arguments, optional*) Additional options for sklearn. model\_selection.GridSearchCV.

#### Raises

**ValueError** – Final regressor does not supply the attributes best\_estimator\_ or best\_params\_.

# property group\_attributes

Group attributes of the input data.

## Туре

numpy.ndarray

# property label

Label of the input data.

Type

str

#### property label\_units

Units of the label.

Туре

str

property mlr\_model\_type

MLR model type.

Туре

str

# property numerical\_features

Numerical features.

Туре

## numpy.ndarray

# property parameters

Parameters of the complete MLR model pipeline.

Type dict

# plot\_1d\_model(filename=None, n\_points=1000)

Plot lineplot that represents the MLR model.

**Note:** This only works for a model with a single feature.

# **Parameters**

- filename (str, optional (default: '1d\_mlr\_model')) Name of the plot file.
- **n\_points** (*int*, *optional* (*default:* 1000)) Number of sampled points for the single feature (using linear spacing between minimum and maximum value).

### Raises

- sklearn.exceptions.NotFittedError MLR model is not fitted.
- ValueError MLR model is built from more than 1 feature.

## plot\_coefs(filename=None)

Plot linear coefficients of models.

Note: The features plotted here are not necessarily the real input features, but the ones after preprocessing.

Parameters

filename (str, optional (default: 'coefs')) – Name of the plot file.

## plot\_feature\_importance(filename=None, color\_coded=True)

Plot feature importance given by linear coefficients.

Note: The features plotted here are not necessarily the real input features, but the ones after preprocessing.

### **Parameters**

- filename (str, optional (default: 'feature\_importance')) Name of the plot file.
- **color\_coded** (*bool*, *optional* (*default: True*)) If True, mark positive (linear) correlations with red bars and negative (linear) correlations with blue bars. If False, all bars are blue.

### plot\_partial\_dependences(filename=None)

Plot partial dependences for every feature.

### Parameters

```
filename (str, optional (default: 'partial_dependece_{feature}')) -
Name of the plot file.
```

#### Raises

sklearn.exceptions.NotFittedError – MLR model is not fitted.

### plot\_prediction\_errors(filename=None)

Plot predicted vs. true values.

# Parameters

**filename** (*str*, *optional* (*default: 'prediction\_errors'*)) – Name of the plot file.

#### Raises

sklearn.exceptions.NotFittedError – MLR model is not fitted.

## plot\_residuals(filename=None)

Plot residuals of training and test (if available) data.

#### Parameters

**filename** (*str*, *optional* (*default:* '*residuals*')) – Name of the plot file.

#### Raises

**sklearn.exceptions.NotFittedError** – MLR model is not fitted.

### plot\_residuals\_distribution(filename=None)

Plot distribution of residuals of training and test data (KDE).

#### Parameters

**filename** (*str*, *optional* (*default:* '*residuals\_distribution*')) – Name of the plot file.

#### Raises

sklearn.exceptions.NotFittedError – MLR model is not fitted.

#### plot\_residuals\_histogram(filename=None)

Plot histogram of residuals of training and test data.

#### Parameters

**filename** (*str*, *optional* (*default: 'residuals\_histogram'*)) – Name of the plot file.

#### Raises

sklearn.exceptions.NotFittedError – MLR model is not fitted.

#### plot\_scatterplots(filename=None)

Plot scatterplots label vs. feature for every feature.

#### **Parameters**

**filename** (*str*, *optional* (*default:* '*scatterplot\_{feature}*')) - Name of the plot file.

### Raises

sklearn.exceptions.NotFittedError - MLR model is not fitted.

Perform prediction using the MLR model(s) and write \*.nc files.

#### Parameters

- save\_mlr\_model\_error (str or int, optional) Additionally saves estimated squared MLR model error. This error represents the uncertainty of the prediction caused by the MLR model itself and not by errors in the prediction input data (errors in that will be considered by including datasets with var\_type set to prediction\_input\_error and setting save\_propagated\_errors to True). If the option is set to 'test', the (constant) error is estimated as RMSEP using a (hold-out) test data set. Only possible if test data is available, i.e. the option test\_size is not set to False during class initialization. If the option is set to 'logo', the (constant) error is estimated as RMSEP using the group\_attributes. Only possible if group\_datasets\_by\_attributes is given. If the option is set to an integer n (!= 0), the (constant) error is estimated as RMSEP using n-fold cross-validation.
- **save\_lime\_importance** (*bool*, *optional* (*default: False*)) Additionally saves local feature importance given by LIME (Local Interpretable Model-agnostic Explanations).
- **save\_propagated\_errors** (*bool*, *optional* (*default: False*)) Additionally saves propagated errors from prediction\_input\_error datasets. Only possible when these are available.
- **\*\*kwargs** (*keyword arguments*, *optional*) Additional options for the final regressors predict() function.

#### Raises

- **RuntimeError** return\_var and return\_cov are both set to True.
- sklearn.exceptions.NotFittedError MLR model is not fitted.
- ValueError An invalid value for save\_mlr\_model\_error is given.
- ValueError save\_propagated\_errors is True and no prediction\_input\_error data is available.

### print\_correlation\_matrices()

Print correlation matrices for all datasets.

#### print\_regression\_metrics(logo=False)

Print all available regression metrics for training data.

#### Parameters

**logo** (bool, optional (default: False)) – Print regression metrics using sklearn.model\_selection.LeaveOneGroupOut cross-validation. Only possible when group\_datasets\_by\_attributes was given during class initialization.

# property random\_state

Random state instance.

Туре

numpy.random.RandomState

## classmethod register\_mlr\_model(mlr\_model\_type)

Add MLR model (subclass of this class) (decorator).

#### reset\_pipeline()

Reset regressor pipeline.

#### rfecv(\*\*kwargs)

Perform recursive feature elimination using cross-validation.

**Note:** This only works for final estimators that provide information about feature importance either through a coef\_ attribute or through a feature\_importances\_ attribute.

#### Parameters

**\*\*kwargs** (*keyword arguments, optional*) – Additional options for sklearn. feature\_selection.RFECV.

### Raises

**RuntimeError** – Final estimator does not provide coef\_ or feature\_importances\_ attribute.

# test\_normality\_of\_residuals()

Perform Shapiro-Wilk test to normality of residuals.

#### Raises

sklearn.exceptions.NotFittedError – MLR model is not fitted.

### update\_parameters(\*\*params)

Update parameters of the whole pipeline.

**Note:** Parameter names have to be given for each step of the pipeline separated by two underscores, i.e. s\_\_p is the parameter p for step s.

### Parameters

**\*\*params** (keyword arguments, optional) – Parameters for the pipeline which should be updated.

#### Raises

ValueError – Invalid parameter for pipeline given.

## **Random Forest Regression**

Random Forest Regression model.

Use mlr\_model\_type: rfr to use this MLR model in the recipe.

#### Classes:

RFRModel(input\_datasets, \*\*kwargs)

Random Forest Regression model.

class esmvaltool.diag\_scripts.mlr.models.rfr.RFRModel(input\_datasets, \*\*kwargs)

Bases: MLRModel

Random Forest Regression model.

# Attributes:

categorical_features	Categorical features.
data	Input data of the MLR model.
features	Features of the input data.
features_after_preprocessing	Features of the input data after preprocessing.
features_types	Types of the features.
features_units	Units of the features.
fit_kwargs	Keyword arguments for fit().
group_attributes	Group attributes of the input data.
label	Label of the input data.
label_units	Units of the label.
mlr_model_type	MLR model type.
numerical_features	Numerical features.
parameters	Parameters of the complete MLR model pipeline.
random_state	Random state instance.

Methods:

<pre>create(mlr_model_type, *args, **kwargs)</pre>	Create desired MLR model subclass (factory method).
efecv(**kwargs)	Perform exhaustive feature elimination using cross-validation.
<pre>export_prediction_data([filename])</pre>	Export all prediction data contained in <i>selfdata</i> .
<pre>export_training_data([filename])</pre>	Export all training data contained in selfdata.
fit()	Fit MLR model.
<pre>get_ancestors([label, features,])</pre>	Return ancestor files.
<pre>get_data_frame(data_type[, impute_nans])</pre>	Return data frame of specified type.
<pre>get_x_array(data_type[, impute_nans])</pre>	Return x data of specific type.
<pre>get_y_array(data_type[, impute_nans])</pre>	Return y data of specific type.
<pre>grid_search_cv(param_grid, **kwargs)</pre>	Perform exhaustive parameter search using cross-validation.
<pre>plot_1d_model([filename, n_points])</pre>	Plot lineplot that represents the MLR model.
<pre>plot_partial_dependences([filename])</pre>	Plot partial dependences for every feature.
<pre>plot_prediction_errors([filename])</pre>	Plot predicted vs.
<pre>plot_residuals([filename])</pre>	Plot residuals of training and test (if available) data.
<pre>plot_residuals_distribution([filename])</pre>	Plot distribution of residuals of training and test data (KDE).
<pre>plot_residuals_histogram([filename])</pre>	Plot histogram of residuals of training and test data.
<pre>plot_scatterplots([filename])</pre>	Plot scatterplots label vs.
<pre>predict([save_mlr_model_error,])</pre>	Perform prediction using the MLR model(s) and write *.nc files.
<pre>print_correlation_matrices()</pre>	Print correlation matrices for all datasets.
<pre>print_regression_metrics([logo])</pre>	Print all available regression metrics for training data.
<pre>register_mlr_model(mlr_model_type)</pre>	Add MLR model (subclass of this class) (decorator).
reset_pipeline()	Reset regressor pipeline.
<pre>rfecv(**kwargs)</pre>	Perform recursive feature elimination using cross-validation.
<pre>test_normality_of_residuals()</pre>	Perform Shapiro-Wilk test to normality of residuals.
<pre>update_parameters(**params)</pre>	Update parameters of the whole pipeline.

# property categorical\_features

Categorical features.

Туре

numpy.ndarray

classmethod create(mlr\_model\_type, \*args, \*\*kwargs)

Create desired MLR model subclass (factory method).

# property data

Input data of the MLR model.

Type dict

# efecv(\*\*kwargs)

Perform exhaustive feature elimination using cross-validation.

```
**kwargs (keyword arguments, optional) – Additional options for esmvaltool. diag_scripts.mlr. custom_sklearn.cross_val_score_weighted().
```

### export\_prediction\_data(filename=None)

Export all prediction data contained in *self.\_data*.

## Parameters

**filename** (*str*, *optional* (*default: '{data\_type}\_{pred\_name}.csv'*)) – Name of the exported files.

#### export\_training\_data(filename=None)

Export all training data contained in *self.\_data*.

#### **Parameters**

**filename** (*str*, *optional* (*default:* '{*data\_type*}.*csv*')) - Name of the exported files.

### property features

Features of the input data.

Туре

numpy.ndarray

### property features\_after\_preprocessing

Features of the input data after preprocessing.

Туре

numpy.ndarray

## property features\_types

Types of the features.

Type

pandas.Series

## property features\_units

Units of the features.

Туре

pandas.Series

# fit()

Fit MLR model.

**Note:** Specifying keyword arguments for this function is not allowed here since *features\_after\_preprocessing* might be altered by that. Use the keyword argument fit\_kwargs during class initialization instead.

### property fit\_kwargs

Keyword arguments for fit().

Type dict

get\_ancestors(label=True, features=None, prediction\_names=None, prediction\_reference=False)

Return ancestor files.

- label (bool, optional (default: True)) Return label files.
- **features** (*list of str*, *optional* (*default: None*)) Features for which files should be returned. If None, return files for all features.

- **prediction\_names** (list of str, optional (default: None)) Prediction names for which files should be returned. If None, return files for all prediction names.
- prediction\_reference (bool, optional (default: False)) Return prediction\_reference files if available for given prediction\_names.

## Returns

Ancestor files.

# **Return type**

list of str

### Raises

**ValueError** – Invalid feature or prediction\_name given.

#### get\_data\_frame(data\_type, impute\_nans=False)

Return data frame of specified type.

### **Parameters**

- **data\_type** (*str*) Data type to be returned. Must be one of 'all', 'train' or 'test'.
- impute\_nans (bool, optional (default: False)) Impute nans if desired.

#### Returns

Desired data.

## **Return type**

pandas.DataFrame

#### Raises

**TypeError** – data\_type is invalid or data does not exist (e.g. test data is not set).

#### get\_x\_array(data\_type, impute\_nans=False)

Return x data of specific type.

# Parameters

- **data\_type** (*str*) Data type to be returned. Must be one of 'all', 'train' or 'test'.
- impute\_nans (bool, optional (default: False)) Impute nans if desired.

# Returns

Desired data.

# **Return type**

numpy.ndarray

#### Raises

**TypeError** – data\_type is invalid or data does not exist (e.g. test data is not set).

# get\_y\_array(data\_type, impute\_nans=False)

Return y data of specific type.

- **data\_type** (*str*) Data type to be returned. Must be one of 'all', 'train' or 'test'.
- impute\_nans (bool, optional (default: False)) Impute nans if desired.

### Returns

Desired data.

# **Return type**

numpy.ndarray

# Raises

**TypeError** – data\_type is invalid or data does not exist (e.g. test data is not set).

#### grid\_search\_cv(param\_grid, \*\*kwargs)

Perform exhaustive parameter search using cross-validation.

### **Parameters**

- **param\_grid** (*dict or list of dict*) Parameter names (keys) and ranges (values) for the search. Have to be given for each step of the pipeline separated by two underscores, i.e. s\_\_p is the parameter p for step s.
- **\*\*kwargs** (*keyword arguments, optional*) Additional options for sklearn. model\_selection.GridSearchCV.

## Raises

**ValueError** – Final regressor does not supply the attributes best\_estimator\_ or best\_params\_.

### property group\_attributes

Group attributes of the input data.

Туре

numpy.ndarray

# property label

Label of the input data.

Type str

property label\_units

Units of the label.

Туре

str

property mlr\_model\_type

MLR model type.

# Туре

str

# property numerical\_features

Numerical features.

### Туре

numpy.ndarray

### property parameters

Parameters of the complete MLR model pipeline.

Туре

dict

#### plot\_1d\_model(filename=None, n\_points=1000)

Plot lineplot that represents the MLR model.

Note: This only works for a model with a single feature.

# Parameters

- **filename** (str, optional (default: '1d\_mlr\_model')) Name of the plot file.
- **n\_points** (*int*, *optional* (*default:* 1000)) Number of sampled points for the single feature (using linear spacing between minimum and maximum value).

#### Raises

- sklearn.exceptions.NotFittedError MLR model is not fitted.
- ValueError MLR model is built from more than 1 feature.

### plot\_partial\_dependences(filename=None)

Plot partial dependences for every feature.

## Parameters

filename (str, optional (default: 'partial\_dependece\_{feature}')) Name of the plot file.

#### Raises

sklearn.exceptions.NotFittedError – MLR model is not fitted.

# plot\_prediction\_errors(filename=None)

Plot predicted vs. true values.

#### Parameters

**filename** (*str*, *optional* (*default: 'prediction\_errors'*)) – Name of the plot file.

#### Raises

sklearn.exceptions.NotFittedError – MLR model is not fitted.

#### plot\_residuals(filename=None)

Plot residuals of training and test (if available) data.

# Parameters

**filename** (*str*, *optional* (*default:* '*residuals*')) – Name of the plot file.

#### Raises

sklearn.exceptions.NotFittedError – MLR model is not fitted.

## plot\_residuals\_distribution(filename=None)

Plot distribution of residuals of training and test data (KDE).

### **Parameters**

**filename** (*str*, *optional* (*default: 'residuals\_distribution'*)) – Name of the plot file.

#### Raises

sklearn.exceptions.NotFittedError – MLR model is not fitted.

#### plot\_residuals\_histogram(filename=None)

Plot histogram of residuals of training and test data.

### Parameters

**filename** (*str*, *optional* (*default: 'residuals\_histogram'*)) – Name of the plot file.

#### Raises

sklearn.exceptions.NotFittedError – MLR model is not fitted.

#### plot\_scatterplots(filename=None)

Plot scatterplots label vs. feature for every feature.

#### Parameters

**filename** (*str*, *optional* (*default:* '*scatterplot\_{feature}*')) – Name of the plot file.

#### Raises

#### sklearn.exceptions.NotFittedError – MLR model is not fitted.

Perform prediction using the MLR model(s) and write \*.nc files.

#### **Parameters**

- **save\_mlr\_model\_error** (*str or int, optional*) Additionally saves estimated squared MLR model error. This error represents the uncertainty of the prediction caused by the MLR model itself and not by errors in the prediction input data (errors in that will be considered by including datasets with var\_type set to prediction\_input\_error and setting save\_propagated\_errors to True). If the option is set to 'test', the (constant) error is estimated as RMSEP using a (hold-out) test data set. Only possible if test data is available, i.e. the option test\_size is not set to False during class initialization. If the option is set to 'logo', the (constant) error is estimated as RMSEP using the group\_attributes. Only possible if group\_datasets\_by\_attributes is given. If the option is set to an integer n (!= 0), the (constant) error is estimated as RMSEP using n-fold cross-validation.
- **save\_lime\_importance** (*bool*, *optional* (*default: False*)) Additionally saves local feature importance given by LIME (Local Interpretable Model-agnostic Explanations).
- **save\_propagated\_errors** (*bool*, *optional* (*default: False*)) Additionally saves propagated errors from prediction\_input\_error datasets. Only possible when these are available.
- **\*\*kwargs** (*keyword arguments*, *optional*) Additional options for the final regressors predict() function.

#### Raises

- **RuntimeError** return\_var and return\_cov are both set to True.
- sklearn.exceptions.NotFittedError MLR model is not fitted.
- ValueError An invalid value for save\_mlr\_model\_error is given.
- **ValueError** save\_propagated\_errors is True and no prediction\_input\_error data is available.

#### print\_correlation\_matrices()

Print correlation matrices for all datasets.

#### print\_regression\_metrics(logo=False)

Print all available regression metrics for training data.

#### Parameters

**logo** (*bool*, *optional* (*default: False*)) – Print regression metrics using sklearn.model\_selection.LeaveOneGroupOut cross-validation. Only possible when *group\_datasets\_by\_attributes* was given during class initialization.

## property random\_state

Random state instance.

Туре

numpy.random.RandomState

#### classmethod register\_mlr\_model(mlr\_model\_type)

Add MLR model (subclass of this class) (decorator).

### reset\_pipeline()

Reset regressor pipeline.

# rfecv(\*\*kwargs)

Perform recursive feature elimination using cross-validation.

**Note:** This only works for final estimators that provide information about feature importance either through a coef\_ attribute or through a feature\_importances\_ attribute.

#### **Parameters**

```
**kwargs (keyword arguments, optional) - Additional options for sklearn. feature_selection.RFECV.
```

### Raises

**RuntimeError** – Final estimator does not provide coef\_ or feature\_importances\_ attribute.

## test\_normality\_of\_residuals()

Perform Shapiro-Wilk test to normality of residuals.

#### Raises

sklearn.exceptions.NotFittedError – MLR model is not fitted.

### update\_parameters(\*\*params)

Update parameters of the whole pipeline.

**Note:** Parameter names have to be given for each step of the pipeline separated by two underscores, i.e. s\_\_p is the parameter p for step s.

### Parameters

**\*\*params** (keyword arguments, optional) – Parameters for the pipeline which should be updated.

#### Raises

**ValueError** – Invalid parameter for pipeline given.

# **Ridge Regression**

Ridge Regression model.

Use mlr\_model\_type: ridge to use this MLR model in the recipe.

# **Classes:**

*RidgeModel*(input\_datasets, \*\*kwargs)

Ridge Regression model.

class esmvaltool.diag\_scripts.mlr.models.ridge.RidgeModel(input\_datasets, \*\*kwargs)

Bases: LinearModel

Ridge Regression model.

# Attributes:

categorical_features	Categorical features.
data	Input data of the MLR model.
features	Features of the input data.
features_after_preprocessing	Features of the input data after preprocessing.
features_types	Types of the features.
features_units	Units of the features.
fit_kwargs	Keyword arguments for <i>fit(</i> ).
group_attributes	Group attributes of the input data.
label	Label of the input data.
label_units	Units of the label.
mlr_model_type	MLR model type.
numerical_features	Numerical features.
parameters	Parameters of the complete MLR model pipeline.
random_state	Random state instance.

# Methods:

<pre>create(mlr_model_type, *args, **kwargs)</pre>	Create desired MLR model subclass (factory method).
efecv(**kwargs)	Perform exhaustive feature elimination using cross-validation.
<pre>export_prediction_data([filename])</pre>	Export all prediction data contained in <i>selfdata</i> .
<pre>export_training_data([filename])</pre>	Export all training data contained in <i>selfdata</i> .
fit()	Fit MLR model.
<pre>get_ancestors([label, features,])</pre>	Return ancestor files.
<pre>get_data_frame(data_type[, impute_nans])</pre>	Return data frame of specified type.
<pre>get_x_array(data_type[, impute_nans])</pre>	Return x data of specific type.
<pre>get_y_array(data_type[, impute_nans])</pre>	Return y data of specific type.
<pre>grid_search_cv(param_grid, **kwargs)</pre>	Perform exhaustive parameter search using cross-validation.
<pre>plot_1d_model([filename, n_points])</pre>	Plot lineplot that represents the MLR model.
<pre>plot_coefs([filename])</pre>	Plot linear coefficients of models.
<pre>plot_feature_importance([filename, color_coded])</pre>	Plot feature importance given by linear coefficients.
plot_partial_dependences([filename])	Plot partial dependences for every feature.
plot_prediction_errors([filename])	Plot predicted vs.
plot_residuals([filename])	Plot residuals of training and test (if available) data.
plot_residuals_distribution([filename])	Plot distribution of residuals of training and test data (KDE).
<pre>plot_residuals_histogram([filename])</pre>	Plot histogram of residuals of training and test data.
<pre>plot_scatterplots([filename])</pre>	Plot scatterplots label vs.
<pre>predict([save_mlr_model_error,])</pre>	Perform prediction using the MLR model(s) and write *.nc files.
<pre>print_correlation_matrices()</pre>	Print correlation matrices for all datasets.
<pre>print_regression_metrics([logo])</pre>	Print all available regression metrics for training data.
<pre>register_mlr_model(mlr_model_type)</pre>	Add MLR model (subclass of this class) (decorator).
reset_pipeline()	Reset regressor pipeline.
rfecv(**kwargs)	Perform recursive feature elimination using cross-validation.
<pre>test_normality_of_residuals()</pre>	Perform Shapiro-Wilk test to normality of residuals.
<pre>update_parameters(**params)</pre>	Update parameters of the whole pipeline.

# property categorical\_features

Categorical features.

## Туре

numpy.ndarray

classmethod create(mlr\_model\_type, \*args, \*\*kwargs)

Create desired MLR model subclass (factory method).

# property data

Input data of the MLR model.

Type dict

# efecv(\*\*kwargs)

Perform exhaustive feature elimination using cross-validation.

**\*\*kwargs** (*keyword arguments, optional*) – Additional options for esmvaltool. diag\_scripts.mlr. custom\_sklearn.cross\_val\_score\_weighted().

#### export\_prediction\_data(filename=None)

Export all prediction data contained in *self.\_data*.

#### **Parameters**

```
filename (str, optional (default: '{data_type}_{pred_name}.csv')) -
Name of the exported files.
```

#### export\_training\_data(filename=None)

Export all training data contained in *self.\_data*.

#### **Parameters**

```
filename (str, optional (default: '{data_type}.csv')) - Name of the exported files.
```

#### property features

Features of the input data.

#### Туре

numpy.ndarray

### property features\_after\_preprocessing

Features of the input data after preprocessing.

#### Туре

numpy.ndarray

#### property features\_types

Types of the features.

#### Туре

pandas.Series

## property features\_units

Units of the features.

# Туре

pandas.Series

#### fit()

Fit MLR model.

**Note:** Specifying keyword arguments for this function is not allowed here since *features\_after\_preprocessing* might be altered by that. Use the keyword argument *fit\_kwargs* during class initialization instead.

#### property fit\_kwargs

Keyword arguments for fit().

Туре

dict

get\_ancestors(label=True, features=None, prediction\_names=None, prediction\_reference=False)
Return ancestor files.

- label (bool, optional (default: True)) Return label files.
- **features** (*list of str*, *optional* (*default: None*)) Features for which files should be returned. If None, return files for all features.
- **prediction\_names** (*list of str, optional (default: None*)) Prediction names for which files should be returned. If None, return files for all prediction names.
- **prediction\_reference** (*bool*, *optional* (*default: False*)) Return prediction\_reference files if available for given prediction\_names.

### Returns

Ancestor files.

#### **Return type**

list of str

### Raises

ValueError – Invalid feature or prediction\_name given.

### get\_data\_frame(data\_type, impute\_nans=False)

Return data frame of specified type.

### **Parameters**

- **data\_type** (*str*) Data type to be returned. Must be one of 'all', 'train' or 'test'.
- impute\_nans (bool, optional (default: False)) Impute nans if desired.

### Returns

Desired data.

#### **Return type**

pandas.DataFrame

# Raises

**TypeError** – data\_type is invalid or data does not exist (e.g. test data is not set).

#### get\_x\_array(data\_type, impute\_nans=False)

Return x data of specific type.

#### Parameters

- **data\_type** (*str*) Data type to be returned. Must be one of 'all', 'train' or 'test'.
- impute\_nans (bool, optional (default: False)) Impute nans if desired.

#### Returns

Desired data.

# **Return type**

numpy.ndarray

## Raises

**TypeError** – data\_type is invalid or data does not exist (e.g. test data is not set).

#### get\_y\_array(data\_type, impute\_nans=False)

Return y data of specific type.

- **data\_type** (*str*) Data type to be returned. Must be one of 'all', 'train' or 'test'.
- impute\_nans (bool, optional (default: False)) Impute nans if desired.

### Returns

Desired data.

# **Return type**

numpy.ndarray

### Raises

TypeError – data\_type is invalid or data does not exist (e.g. test data is not set).

### grid\_search\_cv(param\_grid, \*\*kwargs)

Perform exhaustive parameter search using cross-validation.

### **Parameters**

- **param\_grid** (*dict or list of dict*) Parameter names (keys) and ranges (values) for the search. Have to be given for each step of the pipeline separated by two underscores, i.e. s\_\_p is the parameter p for step s.
- **\*\*kwargs** (*keyword arguments, optional*) Additional options for sklearn. model\_selection.GridSearchCV.

#### Raises

**ValueError** – Final regressor does not supply the attributes best\_estimator\_ or best\_params\_.

# property group\_attributes

Group attributes of the input data.

# Туре

numpy.ndarray

property label

Label of the input data.

Type str

property label\_units

Units of the label.

# Туре

str

## property mlr\_model\_type

MLR model type.

# Туре

str

# property numerical\_features

Numerical features.

### Туре

numpy.ndarray

#### property parameters

Parameters of the complete MLR model pipeline.

Туре

# dict

```
plot_1d_model(filename=None, n_points=1000)
```

Plot lineplot that represents the MLR model.

Note: This only works for a model with a single feature.

### **Parameters**

- **filename** (*str*, *optional* (*default:* '1d\_mlr\_model')) Name of the plot file.
- **n\_points** (*int*, *optional* (*default:* 1000)) Number of sampled points for the single feature (using linear spacing between minimum and maximum value).

#### Raises

- sklearn.exceptions.NotFittedError MLR model is not fitted.
- ValueError MLR model is built from more than 1 feature.

#### plot\_coefs(filename=None)

Plot linear coefficients of models.

Note: The features plotted here are not necessarily the real input features, but the ones after preprocessing.

### Parameters

filename (str, optional (default: 'coefs')) – Name of the plot file.

plot\_feature\_importance(filename=None, color\_coded=True)

Plot feature importance given by linear coefficients.

Note: The features plotted here are not necessarily the real input features, but the ones after preprocessing.

#### **Parameters**

- filename (str, optional (default: 'feature\_importance')) Name of the plot file.
- **color\_coded** (*bool*, *optional* (*default: True*)) If True, mark positive (linear) correlations with red bars and negative (linear) correlations with blue bars. If False, all bars are blue.

#### plot\_partial\_dependences(filename=None)

Plot partial dependences for every feature.

```
filename (str, optional (default: 'partial_dependece_{feature}')) -
Name of the plot file.
```

#### Raises

sklearn.exceptions.NotFittedError – MLR model is not fitted.

#### plot\_prediction\_errors(filename=None)

Plot predicted vs. true values.

### Parameters

**filename**(*str*, *optional* (*default: 'prediction\_errors'*)) – Name of the plot file.

Raises

**sklearn.exceptions.NotFittedError** – MLR model is not fitted.

### plot\_residuals(filename=None)

Plot residuals of training and test (if available) data.

### Parameters

**filename** (*str*, *optional* (*default:* '*residuals*')) – Name of the plot file.

#### Raises

sklearn.exceptions.NotFittedError – MLR model is not fitted.

#### plot\_residuals\_distribution(filename=None)

Plot distribution of residuals of training and test data (KDE).

#### **Parameters**

**filename** (*str*, *optional* (*default:* '*residuals\_distribution*')) – Name of the plot file.

#### Raises

sklearn.exceptions.NotFittedError - MLR model is not fitted.

### plot\_residuals\_histogram(filename=None)

Plot histogram of residuals of training and test data.

#### Parameters

**filename** (*str*, *optional* (*default: 'residuals\_histogram'*)) – Name of the plot file.

#### Raises

sklearn.exceptions.NotFittedError - MLR model is not fitted.

#### plot\_scatterplots(filename=None)

Plot scatterplots label vs. feature for every feature.

#### Parameters

filename (str, optional (default: 'scatterplot\_{feature}')) - Name of
the plot file.

Raises

sklearn.exceptions.NotFittedError – MLR model is not fitted.

## 

Perform prediction using the MLR model(s) and write \*.nc files.

#### **Parameters**

• **save\_mlr\_model\_error** (*str or int, optional*) – Additionally saves estimated squared MLR model error. This error represents the uncertainty of the prediction caused by the MLR model itself and not by errors in the prediction input data (errors in that will be considered by including datasets with var\_type set to prediction\_input\_error and setting save\_propagated\_errors to True). If the option is set to 'test', the (constant) error is estimated as RMSEP using a (hold-out) test data set. Only possible if test data is available, i.e. the option test\_size is not set to False during class initialization. If the option is set to 'logo', the (constant) error is estimated as RMSEP using leave-one-group-out cross-validation using the group\_attributes. Only possible if group\_datasets\_by\_attributes is given. If the option is set to an integer n (!= 0), the (constant) error is estimated as RMSEP using n-fold cross-validation.

- **save\_lime\_importance** (*bool*, *optional* (*default: False*)) Additionally saves local feature importance given by LIME (Local Interpretable Model-agnostic Explanations).
- **save\_propagated\_errors** (*bool*, *optional* (*default: False*)) Additionally saves propagated errors from prediction\_input\_error datasets. Only possible when these are available.
- **\*\*kwargs** (*keyword arguments*, *optional*) Additional options for the final regressors predict() function.

### Raises

- RuntimeError return\_var and return\_cov are both set to True.
- sklearn.exceptions.NotFittedError MLR model is not fitted.
- ValueError An invalid value for save\_mlr\_model\_error is given.
- **ValueError** save\_propagated\_errors is True and no prediction\_input\_error data is available.

### print\_correlation\_matrices()

Print correlation matrices for all datasets.

### print\_regression\_metrics(logo=False)

Print all available regression metrics for training data.

### **Parameters**

**logo** (bool, optional (default: False)) – Print regression metrics using sklearn.model\_selection.LeaveOneGroupOut cross-validation. Only possible when group\_datasets\_by\_attributes was given during class initialization.

### property random\_state

Random state instance.

# Туре

numpy.random.RandomState

# classmethod register\_mlr\_model(mlr\_model\_type)

Add MLR model (subclass of this class) (decorator).

### reset\_pipeline()

Reset regressor pipeline.

# rfecv(\*\*kwargs)

Perform recursive feature elimination using cross-validation.

**Note:** This only works for final estimators that provide information about feature importance either through a coef\_ attribute or through a feature\_importances\_ attribute.

### **Parameters**

```
**kwargs (keyword arguments, optional) - Additional options for sklearn. feature_selection.RFECV.
```

#### Raises

**RuntimeError** – Final estimator does not provide coef\_ or feature\_importances\_ attribute.

### test\_normality\_of\_residuals()

Perform Shapiro-Wilk test to normality of residuals.

### Raises

sklearn.exceptions.NotFittedError – MLR model is not fitted.

# update\_parameters(\*\*params)

Update parameters of the whole pipeline.

**Note:** Parameter names have to be given for each step of the pipeline separated by two underscores, i.e. s\_\_p is the parameter p for step s.

### **Parameters**

**\*\*params** (keyword arguments, optional) – Parameters for the pipeline which should be updated.

#### Raises

**ValueError** – Invalid parameter for pipeline given.

### **Ridge Regression with built-in CV**

Ridge Regression model with built-in CV.

Use mlr\_model\_type: ridge\_cv to use this MLR model in the recipe.

### **Classes:**

*RidgeCVMode1*(input\_datasets, \*\*kwargs) Ridge Regression model with built-in CV.

class esmvaltool.diag\_scripts.mlr.models.ridge\_cv.RidgeCVModel(input\_datasets, \*\*kwargs)
Bases: LinearModel

Ridge Regression model with built-in CV.

Attributes:

categorical_features	Categorical features.
data	Input data of the MLR model.
features	Features of the input data.
features_after_preprocessing	Features of the input data after preprocessing.
features_types	Types of the features.
features_units	Units of the features.
fit_kwargs	Keyword arguments for fit().
group_attributes	Group attributes of the input data.
label	Label of the input data.
label_units	Units of the label.
mlr_model_type	MLR model type.
numerical_features	Numerical features.
parameters	Parameters of the complete MLR model pipeline.
random_state	Random state instance.

# Methods:

<pre>create(mlr_model_type, *args, **kwargs)</pre>	Create desired MLR model subclass (factory method).
efecv(**kwargs)	Perform exhaustive feature elimination using cross-validation.
<pre>export_prediction_data([filename])</pre>	Export all prediction data contained in <i>selfdata</i> .
<pre>export_training_data([filename])</pre>	Export all training data contained in <i>selfdata</i> .
<pre>fit()</pre>	Print final alpha after successful fitting.
<pre>get_ancestors([label, features,])</pre>	Return ancestor files.
<pre>get_data_frame(data_type[, impute_nans])</pre>	Return data frame of specified type.
<pre>get_x_array(data_type[, impute_nans])</pre>	Return x data of specific type.
<pre>get_y_array(data_type[, impute_nans])</pre>	Return y data of specific type.
<pre>grid_search_cv(param_grid, **kwargs)</pre>	Perform exhaustive parameter search using cross-validation.
<pre>plot_1d_model([filename, n_points])</pre>	Plot lineplot that represents the MLR model.
<pre>plot_coefs([filename])</pre>	Plot linear coefficients of models.
<pre>plot_feature_importance([filename,</pre>	Plot feature importance given by linear coefficients.
color_coded])	
<pre>plot_partial_dependences([filename])</pre>	Plot partial dependences for every feature.
<pre>plot_prediction_errors([filename])</pre>	Plot predicted vs.
<pre>plot_residuals([filename])</pre>	Plot residuals of training and test (if available) data.
<pre>plot_residuals_distribution([filename])</pre>	Plot distribution of residuals of training and test data (KDE).
<pre>plot_residuals_histogram([filename])</pre>	Plot histogram of residuals of training and test data.
<pre>plot_scatterplots([filename])</pre>	Plot scatterplots label vs.
<pre>predict([save_mlr_model_error,])</pre>	Perform prediction using the MLR model(s) and write *.nc files.
<pre>print_correlation_matrices()</pre>	Print correlation matrices for all datasets.
<pre>print_regression_metrics([logo])</pre>	Print all available regression metrics for training data.
<pre>register_mlr_model(mlr_model_type)</pre>	Add MLR model (subclass of this class) (decorator).
reset_pipeline()	Reset regressor pipeline.
rfecv(**kwargs)	Perform recursive feature elimination using cross-validation.
<pre>test_normality_of_residuals()</pre>	Perform Shapiro-Wilk test to normality of residuals.
update_parameters(**params)	Update parameters of the whole pipeline.

### property categorical\_features

Categorical features.

Туре

numpy.ndarray

```
classmethod create(mlr_model_type, *args, **kwargs)
```

Create desired MLR model subclass (factory method).

### property data

Input data of the MLR model.

Туре

dict

# efecv(\*\*kwargs)

Perform exhaustive feature elimination using cross-validation.

### Parameters

```
**kwargs (keyword arguments, optional) – Additional options for esmvaltool. diag_scripts.mlr. custom_sklearn.cross_val_score_weighted().
```

### export\_prediction\_data(filename=None)

Export all prediction data contained in *self.\_data*.

### Parameters

```
filename (str, optional (default: '{data_type}_{pred_name}.csv')) -
Name of the exported files.
```

## export\_training\_data(filename=None)

Export all training data contained in *self.\_data*.

#### Parameters

```
filename (str, optional (default: '{data_type}.csv')) - Name of the exported files.
```

# property features

Features of the input data.

Туре

numpy.ndarray

## property features\_after\_preprocessing

Features of the input data after preprocessing.

### Type

numpy.ndarray

# property features\_types

Types of the features.

Туре

pandas.Series

property features\_units

Units of the features.

Туре

pandas.Series

# fit()

Print final alpha after successful fitting.

### property fit\_kwargs

Keyword arguments for *fit(*).

### Туре

dict

get\_ancestors(label=True, features=None, prediction\_names=None, prediction\_reference=False)
Return ancestor files.

### Parameters

- label (bool, optional (default: True)) Return label files.
- **features** (*list of str*, *optional* (*default: None*)) Features for which files should be returned. If None, return files for all features.
- prediction\_names (list of str, optional (default: None)) Prediction names for which files should be returned. If None, return files for all prediction names.
- **prediction\_reference** (bool, optional (default: False)) Return prediction\_reference files if available for given prediction\_names.

#### Returns

Ancestor files.

Return type

list of str

### Raises

**ValueError** – Invalid feature or prediction\_name given.

### get\_data\_frame(data\_type, impute\_nans=False)

Return data frame of specified type.

# Parameters

- **data\_type** (*str*) Data type to be returned. Must be one of 'all', 'train' or 'test'.
- impute\_nans (bool, optional (default: False)) Impute nans if desired.

#### Returns

Desired data.

### **Return type**

pandas.DataFrame

### Raises

**TypeError** – data\_type is invalid or data does not exist (e.g. test data is not set).

#### get\_x\_array(data\_type, impute\_nans=False)

Return x data of specific type.

- **data\_type** (*str*) Data type to be returned. Must be one of 'all', 'train' or 'test'.
- impute\_nans (bool, optional (default: False)) Impute nans if desired.

### Returns

Desired data.

# **Return type**

numpy.ndarray

# Raises

**TypeError** – data\_type is invalid or data does not exist (e.g. test data is not set).

#### get\_y\_array(data\_type, impute\_nans=False)

Return y data of specific type.

### Parameters

- **data\_type** (*str*) Data type to be returned. Must be one of 'all', 'train' or 'test'.
- impute\_nans (bool, optional (default: False)) Impute nans if desired.

#### Returns

Desired data.

# Return type

numpy.ndarray

#### Raises

**TypeError** – data\_type is invalid or data does not exist (e.g. test data is not set).

### grid\_search\_cv(param\_grid, \*\*kwargs)

Perform exhaustive parameter search using cross-validation.

#### **Parameters**

- **param\_grid** (*dict or list of dict*) Parameter names (keys) and ranges (values) for the search. Have to be given for each step of the pipeline separated by two underscores, i.e. s\_\_p is the parameter p for step s.
- **\*\*kwargs** (*keyword arguments, optional*) Additional options for sklearn. model\_selection.GridSearchCV.

### Raises

**ValueError** – Final regressor does not supply the attributes best\_estimator\_ or best\_params\_.

### property group\_attributes

Group attributes of the input data.

### Type

numpy.ndarray

# property label

Label of the input data.

Type str

property label\_units

Units of the label.

Туре

str

#### property mlr\_model\_type

MLR model type.

Туре

str

### property numerical\_features

Numerical features.

Type

# numpy.ndarray

# property parameters

Parameters of the complete MLR model pipeline.

# Туре

dict

# plot\_1d\_model(filename=None, n\_points=1000)

Plot lineplot that represents the MLR model.

Note: This only works for a model with a single feature.

### **Parameters**

- **filename** (*str*, *optional* (*default: '1d\_mlr\_model'*)) Name of the plot file.
- **n\_points** (*int*, *optional* (*default:* 1000)) Number of sampled points for the single feature (using linear spacing between minimum and maximum value).

### Raises

- sklearn.exceptions.NotFittedError MLR model is not fitted.
- ValueError MLR model is built from more than 1 feature.

## plot\_coefs(filename=None)

Plot linear coefficients of models.

Note: The features plotted here are not necessarily the real input features, but the ones after preprocessing.

# Parameters

filename (str, optional (default: 'coefs')) – Name of the plot file.

plot\_feature\_importance(filename=None, color\_coded=True)

Plot feature importance given by linear coefficients.

Note: The features plotted here are not necessarily the real input features, but the ones after preprocessing.

## **Parameters**

• filename (str, optional (default: 'feature\_importance')) - Name of the plot file.

• **color\_coded** (*bool*, *optional* (*default: True*)) – If True, mark positive (linear) correlations with red bars and negative (linear) correlations with blue bars. If False, all bars are blue.

plot\_partial\_dependences(filename=None)

Plot partial dependences for every feature.

# Parameters

```
filename (str, optional (default: 'partial_dependece_{feature}')) - Name of the plot file.
```

Raises

sklearn.exceptions.NotFittedError - MLR model is not fitted.

#### plot\_prediction\_errors(filename=None)

Plot predicted vs. true values.

# Parameters

**filename** (*str*, *optional* (*default:* '*prediction\_errors*')) – Name of the plot file.

Raises

sklearn.exceptions.NotFittedError – MLR model is not fitted.

#### plot\_residuals(filename=None)

Plot residuals of training and test (if available) data.

#### **Parameters**

**filename** (*str*, *optional* (*default:* '*residuals*')) – Name of the plot file.

#### Raises

sklearn.exceptions.NotFittedError – MLR model is not fitted.

### plot\_residuals\_distribution(filename=None)

Plot distribution of residuals of training and test data (KDE).

#### Parameters

**filename** (*str*, *optional* (*default:* '*residuals\_distribution*')) – Name of the plot file.

#### Raises

sklearn.exceptions.NotFittedError – MLR model is not fitted.

#### plot\_residuals\_histogram(filename=None)

Plot histogram of residuals of training and test data.

### Parameters

**filename** (*str*, *optional* (*default:* '*residuals\_histogram*')) – Name of the plot file.

## Raises

sklearn.exceptions.NotFittedError – MLR model is not fitted.

### plot\_scatterplots(filename=None)

Plot scatterplots label vs. feature for every feature.

# Parameters

filename (str, optional (default: 'scatterplot\_{feature}')) - Name of
the plot file.

#### Raises

sklearn.exceptions.NotFittedError – MLR model is not fitted.

Perform prediction using the MLR model(s) and write \*.nc files.

### Parameters

- save\_mlr\_model\_error (str or int, optional) Additionally saves estimated squared MLR model error. This error represents the uncertainty of the prediction caused by the MLR model itself and not by errors in the prediction input data (errors in that will be considered by including datasets with var\_type set to prediction\_input\_error and setting save\_propagated\_errors to True). If the option is set to 'test', the (constant) error is estimated as RMSEP using a (hold-out) test data set. Only possible if test data is available, i.e. the option test\_size is not set to False during class initialization. If the option is set to 'logo', the (constant) error is estimated as RMSEP using the group\_attributes. Only possible if group\_datasets\_by\_attributes is given. If the option is set to an integer n (!= 0), the (constant) error is estimated as RMSEP using n-fold cross-validation.
- **save\_lime\_importance** (*bool*, *optional* (*default: False*)) Additionally saves local feature importance given by LIME (Local Interpretable Model-agnostic Explanations).
- **save\_propagated\_errors** (*bool*, *optional* (*default: False*)) Additionally saves propagated errors from prediction\_input\_error datasets. Only possible when these are available.
- **\*\*kwargs** (*keyword arguments*, *optional*) Additional options for the final regressors predict() function.

### Raises

- RuntimeError return\_var and return\_cov are both set to True.
- sklearn.exceptions.NotFittedError MLR model is not fitted.
- ValueError An invalid value for save\_mlr\_model\_error is given.
- **ValueError** save\_propagated\_errors is True and no prediction\_input\_error data is available.

#### print\_correlation\_matrices()

Print correlation matrices for all datasets.

## print\_regression\_metrics(logo=False)

Print all available regression metrics for training data.

#### Parameters

**logo** (bool, optional (default: False)) – Print regression metrics using sklearn.model\_selection.LeaveOneGroupOut cross-validation. Only possible when group\_datasets\_by\_attributes was given during class initialization.

## property random\_state

Random state instance.

Туре

numpy.random.RandomState

#### classmethod register\_mlr\_model(mlr\_model\_type)

Add MLR model (subclass of this class) (decorator).

#### reset\_pipeline()

Reset regressor pipeline.

#### rfecv(\*\*kwargs)

Perform recursive feature elimination using cross-validation.

**Note:** This only works for final estimators that provide information about feature importance either through a coef\_ attribute or through a feature\_importances\_ attribute.

#### **Parameters**

```
**kwargs (keyword arguments, optional) - Additional options for sklearn. feature_selection.RFECV.
```

#### Raises

**RuntimeError** – Final estimator does not provide coef\_ or feature\_importances\_ attribute.

#### test\_normality\_of\_residuals()

Perform Shapiro-Wilk test to normality of residuals.

#### Raises

sklearn.exceptions.NotFittedError – MLR model is not fitted.

#### update\_parameters(\*\*params)

Update parameters of the whole pipeline.

**Note:** Parameter names have to be given for each step of the pipeline separated by two underscores, i.e. s\_\_p is the parameter p for step s.

#### **Parameters**

**\*\*params** (keyword arguments, optional) – Parameters for the pipeline which should be updated.

#### Raises

**ValueError** – Invalid parameter for pipeline given.

## **Support Vector Regression**

Support Vector Regression model.

Use mlr\_model\_type: svr to use this MLR model in the recipe.

#### **Classes:**

SVRModel(input\_datasets, \*\*kwargs)

Support Vector Regression model.

class esmvaltool.diag\_scripts.mlr.models.svr.SVRModel(input\_datasets, \*\*kwargs)

Bases: MLRModel

Support Vector Regression model.

## Attributes:

categorical_features	Categorical features.
data	Input data of the MLR model.
features	Features of the input data.
features_after_preprocessing	Features of the input data after preprocessing.
features_types	Types of the features.
features_units	Units of the features.
fit_kwargs	Keyword arguments for fit().
group_attributes	Group attributes of the input data.
label	Label of the input data.
label_units	Units of the label.
mlr_model_type	MLR model type.
numerical_features	Numerical features.
parameters	Parameters of the complete MLR model pipeline.
random_state	Random state instance.

## Methods:

<pre>create(mlr_model_type, *args, **kwargs)</pre>	Create desired MLR model subclass (factory method).
efecv(**kwargs)	Perform exhaustive feature elimination using cross-validation.
<pre>export_prediction_data([filename])</pre>	Export all prediction data contained in <i>selfdata</i> .
<pre>export_training_data([filename])</pre>	Export all training data contained in <i>selfdata</i> .
fit()	Fit MLR model.
<pre>get_ancestors([label, features,])</pre>	Return ancestor files.
<pre>get_data_frame(data_type[, impute_nans])</pre>	Return data frame of specified type.
<pre>get_x_array(data_type[, impute_nans])</pre>	Return x data of specific type.
<pre>get_y_array(data_type[, impute_nans])</pre>	Return y data of specific type.
<pre>grid_search_cv(param_grid, **kwargs)</pre>	Perform exhaustive parameter search using cross-validation.
<pre>plot_1d_model([filename, n_points])</pre>	Plot lineplot that represents the MLR model.
<pre>plot_partial_dependences([filename])</pre>	Plot partial dependences for every feature.
<pre>plot_prediction_errors([filename])</pre>	Plot predicted vs.
<pre>plot_residuals([filename])</pre>	Plot residuals of training and test (if available) data.
<pre>plot_residuals_distribution([filename])</pre>	Plot distribution of residuals of training and test data (KDE).
<pre>plot_residuals_histogram([filename])</pre>	Plot histogram of residuals of training and test data.
<pre>plot_scatterplots([filename])</pre>	Plot scatterplots label vs.
<pre>predict([save_mlr_model_error,])</pre>	Perform prediction using the MLR model(s) and write *.nc files.
<pre>print_correlation_matrices()</pre>	Print correlation matrices for all datasets.
<pre>print_regression_metrics([logo])</pre>	Print all available regression metrics for training data.
<pre>register_mlr_model(mlr_model_type)</pre>	Add MLR model (subclass of this class) (decorator).
reset_pipeline()	Reset regressor pipeline.
<pre>rfecv(**kwargs)</pre>	Perform recursive feature elimination using cross-validation.
<pre>test_normality_of_residuals()</pre>	Perform Shapiro-Wilk test to normality of residuals.
<pre>update_parameters(**params)</pre>	Update parameters of the whole pipeline.

## property categorical\_features

Categorical features.

Туре

numpy.ndarray

classmethod create(mlr\_model\_type, \*args, \*\*kwargs)

Create desired MLR model subclass (factory method).

## property data

Input data of the MLR model.

Type dict

## efecv(\*\*kwargs)

Perform exhaustive feature elimination using cross-validation.

## Parameters

**\*\*kwargs** (*keyword arguments, optional*) – Additional options for esmvaltool. diag\_scripts.mlr. custom\_sklearn.cross\_val\_score\_weighted().

## export\_prediction\_data(filename=None)

Export all prediction data contained in *self.\_data*.

## Parameters

**filename** (*str*, *optional* (*default: '{data\_type}\_{pred\_name}.csv'*)) – Name of the exported files.

#### export\_training\_data(filename=None)

Export all training data contained in *self.\_data*.

#### **Parameters**

**filename** (*str*, *optional* (*default:* '{*data\_type*}.*csv*')) - Name of the exported files.

#### property features

Features of the input data.

Туре

numpy.ndarray

#### property features\_after\_preprocessing

Features of the input data after preprocessing.

Туре

numpy.ndarray

## property features\_types

Types of the features.

Type

pandas.Series

#### property features\_units

Units of the features.

Туре

pandas.Series

#### fit()

Fit MLR model.

**Note:** Specifying keyword arguments for this function is not allowed here since *features\_after\_preprocessing* might be altered by that. Use the keyword argument fit\_kwargs during class initialization instead.

#### property fit\_kwargs

Keyword arguments for fit().

Type dict

 $\verb"get_ancestors(label=True, features=None, prediction_names=None, prediction_reference=False)$ 

Return ancestor files.

**Parameters** 

- label (bool, optional (default: True)) Return label files.
- **features** (*list of str*, *optional* (*default: None*)) Features for which files should be returned. If None, return files for all features.

- **prediction\_names** (list of str, optional (default: None)) Prediction names for which files should be returned. If None, return files for all prediction names.
- prediction\_reference (bool, optional (default: False)) Return prediction\_reference files if available for given prediction\_names.

## Returns

Ancestor files.

## **Return type**

list of str

#### Raises

ValueError – Invalid feature or prediction\_name given.

#### get\_data\_frame(data\_type, impute\_nans=False)

Return data frame of specified type.

#### Parameters

- **data\_type** (*str*) Data type to be returned. Must be one of 'all', 'train' or 'test'.
- impute\_nans (bool, optional (default: False)) Impute nans if desired.

#### Returns

Desired data.

## Return type

pandas.DataFrame

#### Raises

**TypeError** – data\_type is invalid or data does not exist (e.g. test data is not set).

#### get\_x\_array(data\_type, impute\_nans=False)

Return x data of specific type.

## Parameters

- **data\_type** (*str*) Data type to be returned. Must be one of 'all', 'train' or 'test'.
- impute\_nans (bool, optional (default: False)) Impute nans if desired.

## Returns

Desired data.

## Return type

numpy.ndarray

#### Raises

**TypeError** – data\_type is invalid or data does not exist (e.g. test data is not set).

## get\_y\_array(data\_type, impute\_nans=False)

Return y data of specific type.

#### Parameters

- **data\_type** (*str*) Data type to be returned. Must be one of 'all', 'train' or 'test'.
- **impute\_nans** (bool, optional (default: False)) Impute nans if desired.

## Returns

Desired data.

## **Return type**

numpy.ndarray

## Raises

**TypeError** – data\_type is invalid or data does not exist (e.g. test data is not set).

#### grid\_search\_cv(param\_grid, \*\*kwargs)

Perform exhaustive parameter search using cross-validation.

#### **Parameters**

- **param\_grid** (*dict or list of dict*) Parameter names (keys) and ranges (values) for the search. Have to be given for each step of the pipeline separated by two underscores, i.e. s\_\_p is the parameter p for step s.
- **\*\*kwargs** (*keyword arguments, optional*) Additional options for sklearn. model\_selection.GridSearchCV.

## Raises

**ValueError** – Final regressor does not supply the attributes best\_estimator\_ or best\_params\_.

## property group\_attributes

Group attributes of the input data.

Туре

numpy.ndarray

## property label

Label of the input data.

# Туре

str

property label\_units

Units of the label.

Type str

# property mlr\_model\_type

MLR model type.

## Туре

str

## property numerical\_features

Numerical features.

## Туре

numpy.ndarray

## property parameters

Parameters of the complete MLR model pipeline.

Туре

dict

#### plot\_1d\_model(filename=None, n\_points=1000)

Plot lineplot that represents the MLR model.

Note: This only works for a model with a single feature.

## Parameters

- filename (str, optional (default: '1d\_mlr\_model')) Name of the plot file.
- **n\_points** (*int*, *optional* (*default:* 1000)) Number of sampled points for the single feature (using linear spacing between minimum and maximum value).

#### Raises

- sklearn.exceptions.NotFittedError MLR model is not fitted.
- ValueError MLR model is built from more than 1 feature.

#### plot\_partial\_dependences(filename=None)

Plot partial dependences for every feature.

## Parameters

filename (str, optional (default: 'partial\_dependece\_{feature}')) Name of the plot file.

#### Raises

sklearn.exceptions.NotFittedError – MLR model is not fitted.

## plot\_prediction\_errors(filename=None)

Plot predicted vs. true values.

#### Parameters

**filename** (*str*, *optional* (*default: 'prediction\_errors'*)) – Name of the plot file.

#### Raises

sklearn.exceptions.NotFittedError – MLR model is not fitted.

#### plot\_residuals(filename=None)

Plot residuals of training and test (if available) data.

#### Parameters

filename (str, optional (default: 'residuals')) – Name of the plot file.

#### Raises

sklearn.exceptions.NotFittedError – MLR model is not fitted.

## plot\_residuals\_distribution(filename=None)

Plot distribution of residuals of training and test data (KDE).

## Parameters

**filename** (*str*, *optional* (*default: 'residuals\_distribution'*)) – Name of the plot file.

#### Raises

sklearn.exceptions.NotFittedError – MLR model is not fitted.

#### plot\_residuals\_histogram(filename=None)

Plot histogram of residuals of training and test data.

#### Parameters

**filename** (*str*, *optional* (*default: 'residuals\_histogram'*)) – Name of the plot file.

#### Raises

sklearn.exceptions.NotFittedError – MLR model is not fitted.

#### plot\_scatterplots(filename=None)

Plot scatterplots label vs. feature for every feature.

#### Parameters

**filename** (*str*, *optional* (*default:* '*scatterplot\_{feature}*')) – Name of the plot file.

#### Raises

#### sklearn.exceptions.NotFittedError – MLR model is not fitted.

Perform prediction using the MLR model(s) and write \*.nc files.

#### **Parameters**

- **save\_mlr\_model\_error** (*str or int, optional*) Additionally saves estimated squared MLR model error. This error represents the uncertainty of the prediction caused by the MLR model itself and not by errors in the prediction input data (errors in that will be considered by including datasets with var\_type set to prediction\_input\_error and setting save\_propagated\_errors to True). If the option is set to 'test', the (constant) error is estimated as RMSEP using a (hold-out) test data set. Only possible if test data is available, i.e. the option test\_size is not set to False during class initialization. If the option is set to 'logo', the (constant) error is estimated as RMSEP using the group\_attributes. Only possible if group\_datasets\_by\_attributes is given. If the option is set to an integer n (!= 0), the (constant) error is estimated as RMSEP using n-fold cross-validation.
- **save\_lime\_importance** (*bool*, *optional* (*default: False*)) Additionally saves local feature importance given by LIME (Local Interpretable Model-agnostic Explanations).
- **save\_propagated\_errors** (*bool*, *optional* (*default: False*)) Additionally saves propagated errors from prediction\_input\_error datasets. Only possible when these are available.
- **\*\*kwargs** (*keyword arguments*, *optional*) Additional options for the final regressors predict() function.

#### Raises

- RuntimeError return\_var and return\_cov are both set to True.
- sklearn.exceptions.NotFittedError MLR model is not fitted.
- ValueError An invalid value for save\_mlr\_model\_error is given.
- **ValueError** save\_propagated\_errors is True and no prediction\_input\_error data is available.

#### print\_correlation\_matrices()

Print correlation matrices for all datasets.

#### print\_regression\_metrics(logo=False)

Print all available regression metrics for training data.

#### Parameters

**logo** (bool, optional (default: False)) – Print regression metrics using sklearn.model\_selection.LeaveOneGroupOut cross-validation. Only possible when group\_datasets\_by\_attributes was given during class initialization.

## property random\_state

Random state instance.

Туре

numpy.random.RandomState

#### classmethod register\_mlr\_model(mlr\_model\_type)

Add MLR model (subclass of this class) (decorator).

#### reset\_pipeline()

Reset regressor pipeline.

## rfecv(\*\*kwargs)

Perform recursive feature elimination using cross-validation.

**Note:** This only works for final estimators that provide information about feature importance either through a coef\_ attribute or through a feature\_importances\_ attribute.

#### **Parameters**

```
**kwargs (keyword arguments, optional) - Additional options for sklearn. feature_selection.RFECV.
```

#### Raises

**RuntimeError** – Final estimator does not provide coef\_ or feature\_importances\_ attribute.

## test\_normality\_of\_residuals()

Perform Shapiro-Wilk test to normality of residuals.

#### Raises

sklearn.exceptions.NotFittedError – MLR model is not fitted.

#### update\_parameters(\*\*params)

Update parameters of the whole pipeline.

**Note:** Parameter names have to be given for each step of the pipeline separated by two underscores, i.e. s\_\_p is the parameter p for step s.

## Parameters

**\*\*params** (keyword arguments, optional) – Parameters for the pipeline which should be updated.

#### Raises

**ValueError** – Invalid parameter for pipeline given.

# 54.3 Monitor Diagnostic

This module provides various tools to monitor climate model simulations. It can be used to plot arbitrary variables from arbitrary datasets.

# 54.3.1 Examples

- Monitor
- General model evaluation

# 54.3.2 Diagnostic scripts

## Monitoring diagnostic to plot arbitrary preprocessor output

Diagnostic to plot preprocessor output.

## **Description**

This diagnostic can be used to visualize arbitrary preprocessor output.

#### Currently supported plot types (use the option plots to specify them):

- Climatology (plot type clim): Plots climatology. Supported coordinates: (*latitude*, *longitude*, *month\_number*).
- Seasonal climatologies (plot type seasonclim): It produces a multi panel (2x2) plot with the seasonal climatologies. Supported coordinates: (*latitude*, *longitude*, *month\_number*).
- Monthly climatologies (plot type monclim): It produces a multi panel (3x4) plot with the monthly climatologies. Can be customized to show only certain months and to rearrange the number of columns and rows. Supported coordinates: (*latitude*, *longitude*, *month\_number*).
- Time series (plot type timeseries): Generate time series plots. It will always generate the full period time series, but if the period is longer than 75 years, it will also generate two extra time series for the first and last 50 years. It will produce multi panel plots for data with *shape\_id* or *region* coordinates of length > 1. Supported coordinates: *time, shape\_id* (optional) and *region* (optional).
- Annual cycle (plot type annual\_cycle): Generate an annual cycle plot (timeseries like climatological from January to December). It will produce multi panel plots for data with *shape\_id* or *region* coordinates of length > 1. Supported coordinates: *time*, *shape\_id* (optional) and *region* (optional).

## **Configuration options in recipe**

#### cartopy\_data\_dir: str, optional (default: None)

Path to cartopy data dir. Defaults to None. See https://scitools.org.uk/cartopy/docs/latest/.

#### config\_file: str, optional

Path to the monitor configuration file. Defaults to monitor\_config.yml in the same folder as the diagnostic script. More information on the monitor configuration file can be found *here*.

#### plots: dict, optional

Plot types plotted by this diagnostic (see list above). Dictionary keys must be clim, seasonclim, monclim,

timeseries or annual\_cycle. Dictionary values are dictionaries used as options for the corresponding plot. The allowed options for the different plot types are given below.

#### plot\_filename: str, optional

Filename pattern for the plots. Defaults to {plot\_type}\_{real\_name}\_{dataset}\_{mip}\_{exp}\_{exsemble}. All tags (i.e., the entries in curly brackets, e.g., {dataset}, are replaced with the corresponding tags).

#### plot\_folder: str, optional

Path to the folder to store figures. Defaults to {plot\_dir}/.././{dataset}/{exp}/{modeling\_realm}/ {real\_name}. All tags (i.e., the entries in curly brackets, e.g., {dataset}, are replaced with the corresponding tags). {plot\_dir} is replaced with the default ESMValTool plot directory (i.e., output\_dir/plots/ diagnostic\_name/script\_name/, see User configuration file).

#### rasterize\_maps: bool, optional (default: True)

If True, use rasterization for map plots to produce smaller files. This is only relevant for vector graphics (e.g., output\_file\_type=pdf,svg,ps).

In the variable definitions, users can set the attribute plot\_name to fix the variable name that will be used for the plot's title. If it is not set, mapgenerator will try to choose a sensible one from the name attributes (long\_name, standard\_name and var\_name).

## Configuration options for plot type clim

#### maps: list of str, optional (default: ['global'])

List of maps to plot, as defined in the monitor configuration file.

## Configuration options for plot type seasonclim

#### maps: list of str, optional (default: ['global'])

List of maps to plot, as defined in the monitor configuration file.

## Configuration options for plot type monclim

#### maps: list of str, optional (default: ['global'])

List of maps to plot, as defined in the monitor configuration file.

#### months: list of int, optional

Select only specific months. Defaults to None (i.e. show all months).

# plot\_size: tuple of int, optional (default: (5, 4)) Size of each individual figure.

# columns: int, optional (default: 3)

Number of columns in the plot.

# rows: int, optional (default: 4)

Number of rows in the plot.

## Configuration options for plot type timeseries

None

## Configuration options for plot type annual\_cycle

None

**Hint:** Extra arguments given to the recipe are ignored, so it is safe to use yaml anchors to share the configuration of common arguments with other monitor diagnostic script.

## Monitoring diagnostic to plot EOF maps and associated PC timeseries

Diagnostic to compute and plot the first EOF of an arbitrary input.

## **Description**

This diagnostic can be used to compute and show Empirical Orthogonal Functions (EOFs) and Principal Components (PCs) of arbitrary input. It creates a map plot of the first EOF and the associated PC time series.

## **Configuration options in recipe**

#### cartopy\_data\_dir: str, optional (default: None)

Path to cartopy data dir. Defaults to None. See https://scitools.org.uk/cartopy/docs/latest/.

#### config\_file: str, optional

Path to the monitor configuration file. Defaults to monitor\_config.yml in the same folder as the diagnostic script. More information on the monitor configuration file can be found *here*.

#### plot\_filename: str, optional

Filename pattern for the plots. Defaults to {plot\_type}\_{real\_name}\_{dataset}\_{mip}\_{exp}\_{ensemble}. All tags (i.e., the entries in curly brackets, e.g., {dataset}, are replaced with the corresponding tags).

## plot\_folder: str, optional

Path to the folder to store figures. Defaults to {plot\_dir}/../.{{dataset}/{exp}/{modeling\_realm}/ {real\_name}. All tags (i.e., the entries in curly brackets, e.g., {dataset}, are replaced with the corresponding tags). {plot\_dir} is replaced with the default ESMValTool plot directory (i.e., output\_dir/plots/ diagnostic\_name/script\_name/, see User configuration file).

#### rasterize\_maps: bool, optional (default: True)

If True, use rasterization for map plots to produce smaller files. This is only relevant for vector graphics (e.g., output\_file\_type=pdf, svg,ps).

**Hint:** Extra arguments given to the recipe are ignored, so it is safe to use yaml anchors to share the configuration of common arguments with other monitor diagnostic script.

## Monitoring diagnostic to show multiple datasets in one plot (incl. biases)

Monitoring diagnostic to show multiple datasets in one plot (incl. biases).

## Description

This diagnostic can be used to visualize multiple datasets in one plot.

For some plot types, a reference dataset can be defined. For this, use the facet reference\_for\_monitor\_diags: true in the definition of the dataset in the recipe. Note that at most one reference dataset per variable is supported.

## Currently supported plot types (use the option plots to specify them):

- Time series (plot type timeseries): for each variable separately, all datasets are plotted in one single figure. Input data needs to be 1D with single dimension *time*.
- Annual cycle (plot type annual\_cycle): for each variable separately, all datasets are plotted in one single figure. Input data needs to be 1D with single dimension *month\_number*.
- Maps (plot type map): for each variable and dataset, an individual map is plotted. If a reference dataset is defined, also include this dataset and a bias plot into the figure. Note that if a reference dataset is defined, all input datasets need to be given on the same horizontal grid (you can use the preprocessor esmvalcore. preprocessor.regrid() for this). Input data needs to be 2D with dimensions *latitude*, *longitude*.
- Zonal mean profiles (plot type zonal\_mean\_profile): for each variable and dataset, an individual profile is plotted. If a reference dataset is defined, also include this dataset and a bias plot into the figure. Note that if a reference dataset is defined, all input datasets need to be given on the same horizontal and vertical grid (you can use the preprocessors esmvalcore.preprocessor.regrid() and esmvalcore. preprocessor.extract\_levels() for this). Input data needs to be 2D with dimensions *latitude*, *altitudelair\_pressure*.

**Warning:** The plot\_type profile for zonal mean profiles has been deprecated in ESMValTool version 2.9.0 and is scheduled for removal in version 2.11.0. Please use plot type zonal\_mean\_profile instead. This is an exact replacement.

- 1D profiles (plot type 1d\_profile): for each variable separately, all datasets are plotted in one single figure. Input data needs to be 1D with single dimension *altitude | air\_pressure*
- Variable vs. latitude plot (plot type variable\_vs\_lat): for each variable separately, all datasets are plotted in one single figure. Input data needs to be 1D with single dimension *latitude*.
- Hovmoeller Z vs. time (plot type hovmoeller\_z\_vs\_time): for each variable and dataset, an individual figure is plotted. If a reference dataset is defined, also include this dataset and a bias plot into the figure. Note that if a reference dataset is defined, all input datasets need to be given on the same temporal and vertical grid (you can use the preprocessors esmvalcore.preprocessor.regrid\_time() and esmvalcore.preprocessor.extract\_levels() for this). Input data needs to be 2D with dimensions time, altitude/air\_pressure.
- Hovmoeller time vs. latitude or longitude (plot type hovmoeller\_time\_vs\_lat\_or\_lon): for each variable and dataset, an individual figure is plotted. If a reference dataset is defined, also include this dataset and a bias plot into the figure. Note that if a reference dataset is defined, all input datasets need to be given on the same temporal and horizontal grid (you can use the preprocessors esmvalcore.preprocessor.regrid\_time() and esmvalcore.preprocessor.regrid() for this). Input data needs to be 2D with dimensions *time*, *latitude/longitude*.

## Author

Manuel Schlund (DLR, Germany)

## **Configuration options in recipe**

#### facet\_used\_for\_labels: str, optional (default: 'dataset')

Facet used to label different datasets in plot titles and legends. For example, facet\_used\_for\_labels: dataset will use dataset names in plot titles and legends; facet\_used\_for\_labels: exp will use experiments in plot titles and legends. In addition, facet\_used\_for\_labels is used to select the correct plot\_kwargs for the different datasets (see configuration options for the different plot types below).

#### figure\_kwargs: dict, optional

Optional keyword arguments for matplotlib.pyplot.figure(). By default, uses constrained\_layout: true.

### group\_variables\_by: str, optional (default: 'short\_name')

Facet which is used to create variable groups. For each variable group, an individual plot is created.

## plots: dict, optional

Plot types plotted by this diagnostic (see list above). Dictionary keys must be timeseries, annual\_cycle, map, zonal\_mean\_profile, 1d\_profile, variable\_vs\_lat, hovmoeller\_z\_vs\_time, hovmoeller\_time\_vs\_lat\_or\_lon. Dictionary values are dictionaries used as options for the corresponding plot. The allowed options for the different plot types are given below.

#### plot\_filename: str, optional

Filename pattern for the plots. Defaults to {plot\_type}\_{real\_name}\_{dataset}\_{mip}\_{exp}\_{ensemble}. All tags (i.e., the entries in curly brackets, e.g., {dataset}, are replaced with the corresponding tags).

## plot\_folder: str, optional

Path to the folder to store figures. Defaults to {plot\_dir}/.././{dataset}/{exp}/{modeling\_realm}/ {real\_name}. All tags (i.e., the entries in curly brackets, e.g., {dataset}, are replaced with the corresponding tags). {plot\_dir} is replaced with the default ESMValTool plot directory (i.e., output\_dir/plots/ diagnostic\_name/script\_name/, see User configuration file).

## savefig\_kwargs: dict, optional

Optional keyword arguments for matplotlib.pyplot.savefig(). By default, uses bbox\_inches: tight, dpi: 300, orientation: landscape.

## seaborn\_settings: dict, optional

Options for seaborn.set\_theme() (affects all plots). By default, uses style: ticks.

#### Configuration options for plot type timeseries

#### annual\_mean\_kwargs: dict, optional

Optional keyword arguments for iris.plot.plot() for plotting annual means. These keyword arguments update (and potentially overwrite) the plot\_kwargs for the annual mean plots. Use annual\_mean\_kwargs to not show annual means.

## gridline\_kwargs: dict, optional

Optional keyword arguments for grid lines. By default, color: lightgrey, alpha: 0.5 are used. Use gridline\_kwargs: false to not show grid lines.

## legend\_kwargs: dict, optional

Optional keyword arguments for matplotlib.pyplot.legend(). Use legend\_kwargs: false to not show legends.

### plot\_kwargs: dict, optional

Optional keyword arguments for iris.plot.plot(). Dictionary keys are elements identified by facet\_used\_for\_labels or default, e.g., CMIP6 if facet\_used\_for\_labels: project or historical if facet\_used\_for\_labels: exp. Dictionary values are dictionaries used as keyword arguments for iris.plot.plot(). String arguments can include facets in curly brackets which will be derived from the corresponding dataset, e.g., {project}, {short\_name}, {exp}. Examples: default: {linestyle: '-', label: '{project}'}, CMIP6: {color: red, linestyle: '--'}, OBS: {color: black}.

## pyplot\_kwargs: dict, optional

Optional calls to functions of matplotlib.pyplot. Dictionary keys are functions of matplotlib. pyplot. Dictionary values are used as single argument for these functions. String arguments can include facets in curly brackets which will be derived from the datasets plotted in the corresponding plot, e.g., {short\_name}, {exp}. Facets like {project} that vary between the different datasets will be transformed to something like ambiguous\_project. Examples: title: 'Awesome Plot of {long\_name}', xlabel: '{short\_name}', xlim: [0, 5].

## time\_format: str, optional (default: None)

strftime() format string that is used to format the time axis using matplotlib.dates.DateFormatter. If
None, use the default formatting imposed by the iris plotting function.

## Configuration options for plot type annual\_cycle

#### gridline\_kwargs: dict, optional

Optional keyword arguments for grid lines. By default, color: lightgrey, alpha: 0.5 are used. Use gridline\_kwargs: false to not show grid lines.

## legend\_kwargs: dict, optional

Optional keyword arguments for matplotlib.pyplot.legend(). Use legend\_kwargs: false to not show legends.

#### plot\_kwargs: dict, optional

Optional keyword arguments for iris.plot.plot(). Dictionary keys are elements identified by facet\_used\_for\_labels or default, e.g., CMIP6 if facet\_used\_for\_labels: project or historical if facet\_used\_for\_labels: exp. Dictionary values are dictionaries used as keyword arguments for iris.plot.plot(). String arguments can include facets in curly brackets which will be derived from the corresponding dataset, e.g., {project}, {short\_name}, {exp}. Examples: default: {linestyle: '-', label: '{project}'}, CMIP6: {color: red, linestyle: '--'}, OBS: {color: black}.

#### pyplot\_kwargs: dict, optional

Optional calls to functions of matplotlib.pyplot. Dictionary keys are functions of matplotlib. pyplot. Dictionary values are used as single argument for these functions. String arguments can include facets in curly brackets which will be derived from the datasets plotted in the corresponding plot, e.g., {short\_name}, {exp}. Facets like {project} that vary between the different datasets will be transformed to something like ambiguous\_project. Examples: title: 'Awesome Plot of {long\_name}', xlabel: '{short\_name}', xlim: [0, 5].

## Configuration options for plot type map

#### cbar\_label: str, optional (default: '{short\_name} [{units}]')

Colorbar label. Can include facets in curly brackets which will be derived from the corresponding dataset, e.g., {project}, {short\_name}, {exp}.

## cbar\_label\_bias: str, optional (default: '{short\_name} [{units}]')

Colorbar label for plotting biases. Can include facets in curly brackets which will be derived from the corresponding dataset, e.g., {project}, {short\_name}, {exp}. This option has no effect if no reference dataset is given.

#### cbar\_kwargs: dict, optional

Optional keyword arguments for matplotlib.pyplot.colorbar(). By default, uses orientation: horizontal, aspect: 30.

#### cbar\_kwargs\_bias: dict, optional

Optional keyword arguments for matplotlib.pyplot.colorbar() for plotting biases. These keyword arguments update (and potentially overwrite) the cbar\_kwargs for the bias plot. This option has no effect if no reference dataset is given.

## common\_cbar: bool, optional (default: False)

Use a common colorbar for the top panels (i.e., plots of the dataset and the corresponding reference dataset) when using a reference dataset. If neither vmin and vmix nor levels is given in plot\_kwargs, the colorbar bounds are inferred from the dataset in the top left panel, which might lead to an inappropriate colorbar for the reference dataset (top right panel). Thus, the use of the plot\_kwargs vmin and vmax or levels is highly recommend when using this common\_cbar: true. This option has no effect if no reference dataset is given.

#### fontsize: int, optional (default: 10)

Fontsize used for ticks, labels and titles. For the latter, use the given fontsize plus 2. Does not affect suptitles.

#### gridline\_kwargs: dict, optional

Optional keyword arguments for grid lines. By default, color: lightgrey, alpha: 0.5 are used. Use gridline\_kwargs: false to not show grid lines.

#### plot\_func: str, optional (default: 'contourf')

Plot function used to plot the maps. Must be a function of iris.plot that supports plotting of 2D cubes with coordinates latitude and longitude.

## plot\_kwargs: dict, optional

Optional keyword arguments for the plot function defined by plot\_func. Dictionary keys are elements identified by facet\_used\_for\_labels or default, e.g., CMIP6 if facet\_used\_for\_labels: project or historical if facet\_used\_for\_labels: exp. Dictionary values are dictionaries used as keyword arguments for the plot function defined by plot\_func. String arguments can include facets in curly brackets which will be derived from the corresponding dataset, e.g., {project}, {short\_name}, {exp}. Examples: default: {levels: 2}, CMIP6: {vmin: 200, vmax: 250}. In addition to the normalization options supported by the plot function, the option norm: centered can be specified. In this case, the keywords vcenter and halfrange should be used instead of vmin or vmax (see CenteredNorm).

#### plot\_kwargs\_bias: dict, optional

Optional keyword arguments for the plot function defined by plot\_func for plotting biases. These keyword arguments update (and potentially overwrite) the plot\_kwargs for the bias plot. This option has no effect if no reference dataset is given. See option plot\_kwargs for more details. By default, uses cmap: bwr and norm: centered.

## projection: str, optional (default: 'Robinson')

Projection used for the map plot. Needs to be a valid projection class of cartopy.crs. Keyword arguments can be specified using the option projection\_kwargs.

## projection\_kwargs: dict, optional

Optional keyword arguments for the projection given by projection. For the default projection Robinson, the default keyword arguments central\_longitude: 10 are used.

## pyplot\_kwargs: dict, optional

Optional calls to functions of matplotlib.pyplot. Dictionary keys are functions of matplotlib.pyplot. Dictionary values are used as single argument for these functions. String arguments can include facets in curly brackets which will be derived from the corresponding dataset, e.g., {project}, {short\_name}, {exp}. Examples: title: 'Awesome Plot of {long\_name}', xlabel: '{short\_name}', xlim: [0, 5].

## rasterize: bool, optional (default: True)

If True, use rasterization for map plots to produce smaller files. This is only relevant for vector graphics (e.g., output\_file\_type: pdf,svg,ps).

## show\_stats: bool, optional (default: True)

Show basic statistics on the plots.

#### x\_pos\_stats\_avg: float, optional (default: 0.0)

Text x-position of average (shown on the left) in Axes coordinates. Can be adjusted to avoid overlap with the figure. Only relevant if show\_stats: true.

## x\_pos\_stats\_bias: float, optional (default: 0.92)

Text x-position of bias statistics (shown on the right) in Axes coordinates. Can be adjusted to avoid overlap with the figure. Only relevant if show\_stats: true.

## Configuration options for plot type zonal\_mean\_profile

## cbar\_label: str, optional (default: '{short\_name} [{units}]')

Colorbar label. Can include facets in curly brackets which will be derived from the corresponding dataset, e.g., {project}, {short\_name}, {exp}.

## cbar\_label\_bias: str, optional (default: '{short\_name} [{units}]')

Colorbar label for plotting biases. Can include facets in curly brackets which will be derived from the corresponding dataset, e.g., {project}, {short\_name}, {exp}. This option has no effect if no reference dataset is given.

## cbar\_kwargs: dict, optional

Optional keyword arguments for matplotlib.pyplot.colorbar(). By default, uses orientation: vertical.

## cbar\_kwargs\_bias: dict, optional

Optional keyword arguments for matplotlib.pyplot.colorbar() for plotting biases. These keyword arguments update (and potentially overwrite) the cbar\_kwargs for the bias plot. This option has no effect if no reference dataset is given.

#### common\_cbar: bool, optional (default: False)

Use a common colorbar for the top panels (i.e., plots of the dataset and the corresponding reference dataset) when using a reference dataset. If neither vmin and vmix nor levels is given in plot\_kwargs, the colorbar bounds are inferred from the dataset in the top left panel, which might lead to an inappropriate colorbar for the reference dataset (top right panel). Thus, the use of the plot\_kwargs vmin and vmax or levels is highly recommend when using this common\_cbar: true. This option has no effect if no reference dataset is given.

#### fontsize: int, optional (default: 10)

Fontsize used for ticks, labels and titles. For the latter, use the given fontsize plus 2. Does not affect suptitles.

#### log\_y: bool, optional (default: True)

Use logarithmic Y-axis.

#### plot\_func: str, optional (default: 'contourf')

Plot function used to plot the profiles. Must be a function of iris.plot that supports plotting of 2D cubes with coordinates latitude and altitude/air\_pressure.

## plot\_kwargs: dict, optional

Optional keyword arguments for the plot function defined by plot\_func. Dictionary keys are elements identified by facet\_used\_for\_labels or default, e.g., CMIP6 if facet\_used\_for\_labels: project or historical if facet\_used\_for\_labels: exp. Dictionary values are dictionaries used as keyword arguments for the plot function defined by plot\_func. String arguments can include facets in curly brackets which will be derived from the corresponding dataset, e.g., {project}, {short\_name}, {exp}. Examples: default: {levels: 2}, CMIP6: {vmin: 200, vmax: 250}. In addition to the normalization options supported by the plot function, the option norm: centered can be specified. In this case, the keywords vcenter and halfrange should be used instead of vmin or vmax (see CenteredNorm).

## plot\_kwargs\_bias: dict, optional

Optional keyword arguments for the plot function defined by plot\_func for plotting biases. These keyword arguments update (and potentially overwrite) the plot\_kwargs for the bias plot. This option has no effect if no reference dataset is given. See option plot\_kwargs for more details. By default, uses cmap: bwr and norm: centered.

## pyplot\_kwargs: dict, optional

Optional calls to functions of matplotlib.pyplot. Dictionary keys are functions of matplotlib.pyplot. Dictionary values are used as single argument for these functions. String arguments can include facets in curly brackets which will be derived from the corresponding dataset, e.g., {project}, {short\_name}, {exp}. Examples: title: 'Awesome Plot of {long\_name}', xlabel: '{short\_name}', xlim: [0, 5].

## rasterize: bool, optional (default: True)

If True, use rasterization for profile plots to produce smaller files. This is only relevant for vector graphics (e.g., output\_file\_type: pdf,svg,ps).

## show\_stats: bool, optional (default: True)

Show basic statistics on the plots.

## show\_y\_minor\_ticklabels: bool, optional (default: False)

Show tick labels for the minor ticks on the Y axis.

## x\_pos\_stats\_avg: float, optional (default: 0.01)

Text x-position of average (shown on the left) in Axes coordinates. Can be adjusted to avoid overlap with the figure. Only relevant if show\_stats: true.

## x\_pos\_stats\_bias: float, optional (default: 0.7)

Text x-position of bias statistics (shown on the right) in Axes coordinates. Can be adjusted to avoid overlap with the figure. Only relevant if show\_stats: true.

## Configuration options for plot type 1d\_profile

#### aspect\_ratio: float, optional (default: 1.5)

Aspect ratio of the plot. The default value results in a slender upright plot.

#### gridline\_kwargs: dict, optional

Optional keyword arguments for grid lines. By default, color: lightgrey, alpha: 0.5 are used. Use gridline\_kwargs: false to not show grid lines.

## legend\_kwargs: dict, optional

Optional keyword arguments for matplotlib.pyplot.legend(). Use legend\_kwargs: false to not show legends.

#### log\_x: bool, optional (default: False)

Use logarithmic X-axis. Note that for the logarithmic x axis tickmarks are set so that minor tickmarks show up. Setting of individual tickmarks by pyplot\_kwargs is not recommended in this case.

#### log\_y: bool, optional (default: True)

Use logarithmic Y-axis.

#### plot\_kwargs: dict, optional

Optional keyword arguments for iris.plot.plot(). Dictionary keys are elements identified by facet\_used\_for\_labels or default, e.g., CMIP6 if facet\_used\_for\_labels: project or historical if facet\_used\_for\_labels: exp. Dictionary values are dictionaries used as keyword arguments for iris.plot.plot(). String arguments can include facets in curly brackets which will be derived from the corresponding dataset, e.g., {project}, {short\_name}, {exp}. Examples: default: {linestyle: '-', label: '{project}'}, CMIP6: {color: red, linestyle: '--'}, OBS: {color: black}.

## pyplot\_kwargs: dict, optional

Optional calls to functions of matplotlib.pyplot. Dictionary keys are functions of matplotlib. pyplot. Dictionary values are used as single argument for these functions. String arguments can include facets in curly brackets which will be derived from the datasets plotted in the corresponding plot, e.g., {short\_name}, {exp}. Facets like {project} that vary between the different datasets will be transformed to something like ambiguous\_project. Examples: title: 'Awesome Plot of {long\_name}', xlabel: '{short\_name}', xlim: [0, 5].

## show\_y\_minor\_ticklabels: bool, optional (default: False)

Show tick labels for the minor ticks on the Y axis.

## Configuration options for plot type variable\_vs\_lat

#### gridline\_kwargs: dict, optional

Optional keyword arguments for grid lines. By default, color: lightgrey, alpha: 0.5 are used. Use gridline\_kwargs: false to not show grid lines.

## legend\_kwargs: dict, optional

Optional keyword arguments for matplotlib.pyplot.legend(). Use legend\_kwargs: false to not show legends.

#### plot\_kwargs: dict, optional

Optional keyword arguments for iris.plot.plot(). Dictionary keys are elements identified by facet\_used\_for\_labels or default, e.g., CMIP6 if facet\_used\_for\_labels: project or historical if facet\_used\_for\_labels: exp. Dictionary values are dictionaries used as keyword arguments for iris.plot.plot(). String arguments can include facets in curly brackets which will be derived from the corresponding dataset, e.g., {project}, {short\_name}, {exp}. Examples: default: {linestyle: '-', label: '{project}'}, CMIP6: {color: red, linestyle: '--'}, OBS: {color: black}.

## pyplot\_kwargs: dict, optional

Optional calls to functions of matplotlib.pyplot. Dictionary keys are functions of matplotlib. pyplot. Dictionary values are used as single argument for these functions. String arguments can include facets in curly brackets which will be derived from the datasets plotted in the corresponding plot, e.g., {short\_name}, {exp}. Facets like {project} that vary between the different datasets will be transformed to something like ambiguous\_project. Examples: title: 'Awesome Plot of {long\_name}', xlabel: '{short\_name}', xlim: [0, 5].

## Configuration options for plot type hovmoeller\_z\_vs\_time

#### cbar\_label: str, optional (default: '{short\_name} [{units}]')

Colorbar label. Can include facets in curly brackets which will be derived from the corresponding dataset, e.g., {project}, {short\_name}, {exp}.

## cbar\_label\_bias: str, optional (default: '{short\_name} [{units}]')

Colorbar label for plotting biases. Can include facets in curly brackets which will be derived from the corresponding dataset, e.g., {project}, {short\_name}, {exp}. This option has no effect if no reference dataset is given.

#### cbar\_kwargs: dict, optional

Optional keyword arguments for matplotlib.pyplot.colorbar(). By default, uses orientation: vertical.

#### cbar\_kwargs\_bias: dict, optional

Optional keyword arguments for matplotlib.pyplot.colorbar() for plotting biases. These keyword arguments update (and potentially overwrite) the cbar\_kwargs for the bias plot. This option has no effect if no reference dataset is given.

## common\_cbar: bool, optional (default: False)

Use a common colorbar for the top panels (i.e., plots of the dataset and the corresponding reference dataset) when using a reference dataset. If neither vmin and vmix nor levels is given in plot\_kwargs, the colorbar bounds are inferred from the dataset in the top left panel, which might lead to an inappropriate colorbar for the reference dataset (top right panel). Thus, the use of the plot\_kwargs vmin and vmax or levels is highly recommend when using this common\_cbar: true. This option has no effect if no reference dataset is given.

#### fontsize: int, optional (default: 10)

Fontsize used for ticks, labels and titles. For the latter, use the given fontsize plus 2. Does not affect suptitles.

#### log\_y: bool, optional (default: True)

Use logarithmic Y-axis.

#### plot\_func: str, optional (default: 'contourf')

Plot function used to plot the profiles. Must be a function of iris.plot that supports plotting of 2D cubes with coordinates latitude and altitude/air\_pressure.

## plot\_kwargs: dict, optional

Optional keyword arguments for the plot function defined by plot\_func. Dictionary keys are elements identified by facet\_used\_for\_labels or default, e.g., CMIP6 if facet\_used\_for\_labels: project or historical if facet\_used\_for\_labels: exp. Dictionary values are dictionaries used as keyword arguments for the plot function defined by plot\_func. String arguments can include facets in curly brackets which will be derived from the corresponding dataset, e.g., {project}, {short\_name}, {exp}. Examples: default: {levels: 2}, CMIP6: {vmin: 200, vmax: 250}. In addition to the normalization options supported by the plot function, the option norm: centered can be specified. In this case, the keywords vcenter and halfrange should be used instead of vmin or vmax (see CenteredNorm).

#### plot\_kwargs\_bias: dict, optional

Optional keyword arguments for the plot function defined by plot\_func for plotting biases. These keyword arguments update (and potentially overwrite) the plot\_kwargs for the bias plot. This option has no effect if no reference dataset is given. See option plot\_kwargs for more details. By default, uses cmap: bwr and norm: centered.

## pyplot\_kwargs: dict, optional

Optional calls to functions of matplotlib.pyplot. Dictionary keys are functions of matplotlib.pyplot. Dictionary values are used as single argument for these functions. String arguments can include facets in curly brackets which will be derived from the corresponding dataset, e.g., {project}, {short\_name}, {exp}. Examples: title: 'Awesome Plot of {long\_name}', xlabel: '{short\_name}', xlim: [0, 5].

#### rasterize: bool, optional (default: True)

If True, use rasterization for profile plots to produce smaller files. This is only relevant for vector graphics (e.g., output\_file\_type: pdf, svg,ps).

#### show\_stats: bool, optional (default: True)

Show basic statistics on the plots.

## show\_y\_minor\_ticklabels: bool, optional (default: False)

Show tick labels for the minor ticks on the Y axis.

## x\_pos\_stats\_avg: float, optional (default: 0.01)

Text x-position of average (shown on the left) in Axes coordinates. Can be adjusted to avoid overlap with the figure. Only relevant if show\_stats: true.

#### x\_pos\_stats\_bias: float, optional (default: 0.7)

Text x-position of bias statistics (shown on the right) in Axes coordinates. Can be adjusted to avoid overlap with the figure. Only relevant if show\_stats: true.

#### time\_format: str, optional (default: None)

strftime() format string that is used to format the time axis using matplotlib.dates.DateFormatter. If
None, use the default formatting imposed by the iris plotting function.

#### Configuration options for plot type hovmoeller\_time\_vs\_lat\_or\_lon

#### cbar\_label: str, optional (default: '{short\_name} [{units}]')

Colorbar label. Can include facets in curly brackets which will be derived from the corresponding dataset, e.g., {project}, {short\_name}, {exp}.

#### cbar\_label\_bias: str, optional (default: '{short\_name} [{units}]')

Colorbar label for plotting biases. Can include facets in curly brackets which will be derived from the corresponding dataset, e.g., {project}, {short\_name}, {exp}. This option has no effect if no reference dataset is given.

#### cbar\_kwargs: dict, optional

Optional keyword arguments for matplotlib.pyplot.colorbar(). By default, uses orientation: vertical.

## cbar\_kwargs\_bias: dict, optional

Optional keyword arguments for matplotlib.pyplot.colorbar() for plotting biases. These keyword arguments update (and potentially overwrite) the cbar\_kwargs for the bias plot. This option has no effect if no reference dataset is given.

## common\_cbar: bool, optional (default: False)

Use a common colorbar for the top panels (i.e., plots of the dataset and the corresponding reference dataset) when using a reference dataset. If neither vmin and vmix nor levels is given in plot\_kwargs, the colorbar bounds are inferred from the dataset in the top left panel, which might lead to an inappropriate colorbar for the reference dataset (top right panel). Thus, the use of the plot\_kwargs vmin and vmax or levels is highly recommend when using this common\_cbar: true. This option has no effect if no reference dataset is given.

## fontsize: int, optional (default: 10)

Fontsize used for ticks, labels and titles. For the latter, use the given fontsize plus 2. Does not affect suptitles.

## plot\_func: str, optional (default: 'contourf')

Plot function used to plot the profiles. Must be a function of iris.plot that supports plotting of 2D cubes with coordinates latitude and height/air\_pressure.

#### plot\_kwargs: dict, optional

Optional keyword arguments for the plot function defined by plot\_func. Dictionary keys are elements identified by facet\_used\_for\_labels or default, e.g., CMIP6 if facet\_used\_for\_labels: project or historical if facet\_used\_for\_labels: exp. Dictionary values are dictionaries used as keyword arguments for the plot function defined by plot\_func. String arguments can include facets in curly brackets which will be derived from the corresponding dataset, e.g., {project}, {short\_name}, {exp}. Examples: default: {levels: 2}, CMIP6: {vmin: 200, vmax: 250}. In addition to the normalization options supported by the plot function, the option norm: centered can be specified. In this case, the keywords vcenter and halfrange should be used instead of vmin or vmax (see CenteredNorm).

## plot\_kwargs\_bias: dict, optional

Optional keyword arguments for the plot function defined by plot\_func for plotting biases. These keyword arguments update (and potentially overwrite) the plot\_kwargs for the bias plot. This option has no effect if no reference dataset is given. See option plot\_kwargs for more details. By default, uses cmap: bwr and norm: centered.

## pyplot\_kwargs: dict, optional

Optional calls to functions of matplotlib.pyplot. Dictionary keys are functions of matplotlib.pyplot. Dictionary values are used as single argument for these functions. String arguments can include facets in curly brackets which will be derived from the corresponding dataset, e.g., {project}, {short\_name}, {exp}. Examples: title: 'Awesome Plot of {long\_name}', xlabel: '{short\_name}', xlim: [0, 5].

#### rasterize: bool, optional (default: True)

If True, use rasterization for profile plots to produce smaller files. This is only relevant for vector graphics (e.g., output\_file\_type: pdf, svg,ps).

## show\_y\_minor\_ticks: bool, optional (default: True)

Show minor ticks for time on the Y axis.

## show\_x\_minor\_ticks: bool, optional (default: True)

Show minor ticks for latitude or longitude on the X axis.

## time\_format: str, optional (default: None)

strftime() format string that is used to format the time axis using matplotlib.dates.DateFormatter. If
None, use the default formatting imposed by the iris plotting function.

**Hint:** Extra arguments given to the recipe are ignored, so it is safe to use yaml anchors to share the configuration of common arguments with other monitor diagnostic script.

# 54.3.3 Base class for monitoring diagnostics

#### Base class for monitoring diagnostics

Base class for monitoring diagnostics.

#### **Classes:**

MonitorBase(config) Base class for monitoring diagnostic.

## class esmvaltool.diag\_scripts.monitor.monitor\_base.MonitorBase(config)

Bases: object

Base class for monitoring diagnostic.

It contains the common methods for path creation, provenance recording, option parsing and to create some common plots.

#### Methods:

<pre>get_plot_folder(var_info)</pre>	Get plot storage folder from variable info.
<pre>get_plot_name(plot_type, var_info[, add_ext])</pre>	Get plot filename from variable info.
<pre>get_plot_path(plot_type, var_info[, add_ext])</pre>	Get plot full path from variable info.
<pre>get_provenance_record(ancestor_files,</pre>	Create provenance record for the diagnostic data and
**kwargs)	plots.
<pre>plot_cube(cube, filename[, linestyle])</pre>	Plot a timeseries from a cube.
<pre>plot_timeseries(cube, var_info[, period])</pre>	Plot timeseries from a cube.
<pre>record_plot_provenance(filename, var_info,)</pre>	Write provenance info for a given file.

## get\_plot\_folder(var\_info)

Get plot storage folder from variable info.

## **Parameters** var\_info (*dict*) – Variable information from ESMValTool

## get\_plot\_name(plot\_type, var\_info, add\_ext=True)

Get plot filename from variable info.

#### Parameters

- plot\_type (str) Name of the plot
- **var\_info** (*dict*) Variable information from ESMValTool
- **add\_ext** (*bool*, *optional* (*default: True*)) Add filename extension from configuration file.

#### get\_plot\_path(plot\_type, var\_info, add\_ext=True)

Get plot full path from variable info.

#### **Parameters**

- plot\_type (str) Name of the plot
- var\_info (dict) Variable information from ESMValTool
- **add\_ext** (*bool*, *optional* (*default: True*)) Add filename extension from configuration file.

## static get\_provenance\_record(ancestor\_files, \*\*kwargs)

Create provenance record for the diagnostic data and plots.

## plot\_cube(cube, filename, linestyle='-', \*\*kwargs)

Plot a timeseries from a cube.

Supports multiplot layouts for cubes with extra dimensions *shape\_id* or *region*.

## plot\_timeseries(cube, var\_info, period=", \*\*kwargs)

Plot timeseries from a cube.

#### It also automatically smoothes it for long timeseries of monthly data:

- Between 10 and 70 years long, it also plots the 12-month rolling average along the raw series
- For more than ten years, it plots the 12-month and 10-years rolling averages and not the raw series

## record\_plot\_provenance(filename, var\_info, plot\_type, \*\*kwargs)

Write provenance info for a given file.

# 54.4 Ocean diagnostics toolkit

Welcome to the API documentation for the ocean diagnostics tool kit. This toolkit is built to assist in the evaluation of models of the ocean.

This toolkit is part of ESMValTool v2.

```
Author: Lee de Mora (PML)
ledm@pml.ac.uk
```

# 54.4.1 Maps diagnostics

Diagnostic to produce images of a map with coastlines from a cube. These plost show latitude vs longitude and the cube value is used as the colour scale.

Note that this diagnostic assumes that the preprocessors do the bulk of the hard work, and that the cube received by this diagnostic (via the settings.yml and metadata.yml files) has no time component, a small number of depth layers, and a latitude and longitude coordinates.

An approproate preprocessor for a 3D+time field would be:

```
preprocessors:
    prep_map:
    extract_levels:
        levels: [100., ]
        scheme: linear_extrap
    climate_statistics:
        operator: mean
```

Note that this recipe may not function on machines with no access to the internet, as cartopy may try to download the shapefiles. The solution to this issue is the put the relevant cartopy shapefiles on a disk visible to your machine, then link that path to ESMValTool via the *auxiliary\_data\_dir* variable. The cartopy masking files can be downloaded from:

```
https://www.naturalearthdata.com/downloads/
```

Here, cartopy uses the 1:10, physical coastlines and land files:

```
110m_coastline.dbf 110m_coastline.shp 110m_coastline.shx
110m_land.dbf 110m_land.shp 110m_land.shx
```

This tool is part of the ocean diagnostic tools package in the ESMValTool.

Author: Lee de Mora (PML)

ledm@pml.ac.uk

## **Functions:**

<pre>main(cfg)</pre>	Load the config file, and send it to the plot makers.
<pre>make_map_contour(cfg, metadata, filename)</pre>	Make a simple contour map plot for an individual model.
<pre>make_map_plots(cfg, metadata, filename)</pre>	Make a simple map plot for an individual model.
<pre>multi_model_contours(cfg, metadata)</pre>	Make a contour map showing several models.

esmvaltool.diag\_scripts.ocean.diagnostic\_maps.main(cfg)

Load the config file, and send it to the plot makers.

#### **Parameters**

**cfg** (*dict*) – the opened global config dictionary, passed by ESMValTool.

esmvaltool.diag\_scripts.ocean.diagnostic\_maps.make\_map\_contour(*cfg*, *metadata*, *filename*) Make a simple contour map plot for an individual model.

#### Parameters

- **cfg** (*dict*) the opened global config dictionary, passed by ESMValTool.
- metadata (dict) the metadata dictionary
- filename (str) the preprocessed model file.

esmvaltool.diag\_scripts.ocean.diagnostic\_maps.make\_map\_plots(cfg, metadata, filename)

Make a simple map plot for an individual model.

#### Parameters

- **cfg** (*dict*) the opened global config dictionary, passed by ESMValTool.
- metadata (dict) the metadata dictionary
- **filename** (*str*) the preprocessed model file.

esmvaltool.diag\_scripts.ocean.diagnostic\_maps.multi\_model\_contours(cfg, metadata)

Make a contour map showing several models.

#### **Parameters**

- **cfg** (*dict*) the opened global config dictionary, passed by ESMValTool.
- metadata (dict) the metadata dictionary.

## 54.4.2 Model 1 vs Model 2 vs Observations diagnostics.

Diagnostic to produce an image showing four maps, based on a comparison of two differnt models results against an observational dataset. This process is often used to compare a new iteration of a model under development against a previous version of the same model. The four map plots are:

- Top left: model 1
- Top right: model 1 minus model 2
- Bottom left: model 2 minus obs
- Bottom right: model 1 minus obs

All four plots show latitude vs longitude and the cube value is used as the colour scale.

Note that this diagnostic assumes that the preprocessors do the bulk of the hard work, and that the cube received by this diagnostic (via the settings.yml and metadata.yml files) has no time component, a small number of depth layers, and a latitude and longitude coordinates.

An approproate preprocessor for a 3D+time field would be:

```
preprocessors:
    prep_map:
    extract_levels:
        levels: [100., ]
        scheme: linear_extrap
        climate_statistics:
        operator: mean
```

This diagnostic also requires the exper\_model, exper\_model and observational\_dataset keys in the recipe:

```
diagnostics:
    diag_name:
        scripts:
        Global_Ocean_map:
            script: ocean/diagnostic_maps_quad.py
            exper_model: {Model 1 dataset details}
            control_model: {Model 2 dataset details}
            observational_dataset: {Observational dataset details}
```

This tool is part of the ocean diagnostic tools package in the ESMValTool, and was based on the plots produced by the Ocean Assess/Marine Assess toolkit.

#### Author: Lee de Mora (PML)

ledm@pml.ac.uk

## **Functions:**

<pre>add_map_subplot(subplot, cube, nspace[,])</pre>	Add a map subplot to the current pyplot figure.
<pre>main(cfg)</pre>	Load the config file, and send it to the plot maker.
<pre>multi_model_maps(cfg, input_files)</pre>	Make the four pane model vs model vs obs comparison
	plot.

Add a map subplot to the current pyplot figure.

#### **Parameters**

- **subplot** (*int*) The matplotlib.pyplot subplot number. (ie 221)
- cube (iris.cube.Cube) the iris cube to be plotted.
- **nspace** (*numpy.array*) An array of the ticks of the colour part.
- **title** (*str*) A string to set as the subplot title.
- **cmap** (*str*) A string to describe the matplotlib colour map.

esmvaltool.diag\_scripts.ocean.diagnostic\_maps\_quad.main(cfg)

Load the config file, and send it to the plot maker.

#### **Parameters**

**cfg** (*dict*) – the opened global config dictionairy, passed by ESMValTool.

esmvaltool.diag\_scripts.ocean.diagnostic\_maps\_quad.multi\_model\_maps(cfg, input\_files)
Make the four pane model vs model vs obs comparison plot.

#### **Parameters**

- **cfg** (*dict*) the opened global config dictionairy, passed by ESMValTool.
- input\_files (dict) the metadata dictionairy

# 54.4.3 Model vs Observations maps Diagnostic.

Diagnostic to produce comparison of model and data. The first kind of image shows four maps and the other shows a scatter plot.

The four pane image is a latitude vs longitude figures showing:

- Top left: model
- Top right: observations
- Bottom left: model minus observations
- Bottom right: model over observations

The scatter plots plot the matched model coordinate on the x axis, and the observational dataset on the y coordinate, then performs a linear regression of those data and plots the line of best fit on the plot. The parameters of the fit are also shown on the figure.

Note that this diagnostic assumes that the preprocessors do the bulk of the hard work, and that the cube received by this diagnostic (via the settings.yml and metadata.yml files) has no time component, a small number of depth layers, and a latitude and longitude coordinates.

An appropriate preprocessor for a 3D + time field would be:

```
preprocessors:
    prep_map:
    extract_levels:
        levels: [100., ]
        scheme: linear_extrap
        climate_statistics:
        operator: mean
        regrid:
        target_grid: 1x1
        scheme: linear
```

This tool is part of the ocean diagnostic tools package in the ESMValTool, and was based on the plots produced by the Ocean Assess/Marine Assess toolkit.

## Author: Lee de Mora (PML)

ledm@pml.ac.uk

#### **Functions:**

<pre>add_linear_regression(plot_axes, arr_x, arr_y)</pre>	Add a straight line fit to an axis.
<pre>add_map_subplot(subplot, cube, nspace[,])</pre>	Add a map subplot to the current pyplot figure.
<pre>main(cfg)</pre>	Load the config file, and send it to the plot maker.
<pre>make_model_vs_obs_plots(cfg, metadata,)</pre>	Make a figure showing four maps and the other shows a scatter plot.
<pre>make_scatter(cfg, metadata, model_filename,)</pre>	Makes Scatter plots of model vs observational data.
<pre>rounds_sig(value[, sig])</pre>	Round a float to sig significant digits & return it as a string.

esmvaltool.diag\_scripts.ocean.diagnostic\_model\_vs\_obs.add\_linear\_regression(plot\_axes, arr\_x,

arr\_y, showtext=True, add\_diagonal=False, extent=None) Add a straight line fit to an axis.

## Parameters

- **plot\_axes** (*matplotlib.pyplot.axes*) The matplotlib axes on which to plot the linear regression.
- **arr\_x** (*numpy.array*) The data for the x coordinate.
- **arr\_y** (*numpy array*) The data for the y coordinate.
- showtext (bool) A flag to turn on or off the result of the fit on the plot.
- add\_diagonal (bool) A flag to also add the 1:1 diagonal line to the figure
- **extent** (*list of floats*) The extent of the plot axes.

esmvaltool.diag\_scripts.ocean.diagnostic\_model\_vs\_obs.add\_map\_subplot(subplot, cube, nspace,

title=", cmap=", extend='neither', log=False)

Add a map subplot to the current pyplot figure.

#### **Parameters**

- **subplot** (*int*) The matplotlib.pyplot subplot number. (ie 221)
- cube (iris.cube.Cube) the iris cube to be plotted.
- **nspace** (*numpy.array*) An array of the ticks of the colour part.
- title (*str*) A string to set as the subplot title.
- **cmap** (*str*) A string to describe the matplotlib colour map.
- extend (str) Contourf-coloring of values outside the levels range
- log (bool) Flag to plot the colour scale linearly (False) or logarithmically (True)

esmvaltool.diag\_scripts.ocean.diagnostic\_model\_vs\_obs.main(cfg)

Load the config file, and send it to the plot maker.

## Parameters

cfg (dict) – the opened global config dictionairy, passed by ESMValTool.

Make a figure showing four maps and the other shows a scatter plot.

The four pane image is a latitude vs longitude figures showing:

- Top left: model
- Top right: observations
- Bottom left: model minus observations
- Bottom right: model over observations

#### **Parameters**

- **cfg** (*dict*) the opened global config dictionairy, passed by ESMValTool.
- metadata (dict) the input files dictionairy

- model\_filename (str) the preprocessed model file.
- **obs\_filename** (*str*) the preprocessed observations file.

obs\_filename)

Makes Scatter plots of model vs observational data.

Make scatter plot showing the matched model and observational data with the model data as the x-axis coordinate and the observational data as the y-axis coordinate. A linear regression is also applied to the matched data and the result of the fit is shown on the figure.

## Parameters

- **cfg** (*dict*) the opened global config dictionairy, passed by ESMValTool.
- metadata (dict) the input files dictionairy
- model\_filename (str) the preprocessed model file.
- **obs\_filename** (*str*) the preprocessed observations file.

esmvaltool.diag\_scripts.ocean.diagnostic\_model\_vs\_obs.rounds\_sig(value, sig=3)
Round a float to sig significant digits & return it as a string.

#### Parameters

- **value** (*float*) The float that is to be rounded.
- **sig** (*int*) The number of significant figures.

#### Returns

The rounded output string.

Return type str

## 54.4.4 Profile diagnostics.

Diagnostic to produce figure of the profile over time from a cube. These plost show cube value (ie temperature) on the x-axis, and depth/height on the y axis. The colour scale is the time series.

Note that this diagnostic assumes that the preprocessors do the bulk of the hard work, and that the cube received by this diagnostic (via the settings.yml and metadata.yml files) has a time component, and depth component, but no latitude or longitude coordinates.

An approproate preprocessor for a 3D+time field would be:

```
preprocessors:
    prep_profile:
        extract_volume:
        long1: 0.
        long2: 20.
        lat1: -30.
        lat2: 30.
        z_min: 0.
        z_max: 3000.
        area_statistics:
        operator: mean
```

In order to add an observational dataset to the profile plot, the following arguments are needed in the diagnostic script:

```
diagnostics:
    diagnostic_name:
        variables:
        ...
    additional_datasets:
        - {observational dataset description}
        scripts:
            script_name:
            script: ocean/diagnostic_profiles.py
            observational_dataset: {observational dataset description}
```

This tool is part of the ocean diagnostic tools package in the ESMValTool.

#### Author: Lee de Mora (PML)

ledm@pml.ac.uk

## **Functions:**

<pre>determine_profiles_str(cube)</pre>	Determine a string from the cube, to describe the profile.
main(cfg)	Run the diagnostics profile tool.
<pre>make_profiles_plots(cfg, metadata, filename)</pre>	Make a profile plot for an individual model.

esmvaltool.diag\_scripts.ocean.diagnostic\_profiles.determine\_profiles\_str(cube)

Determine a string from the cube, to describe the profile.

```
Parameters
cube (iris.cube.Cube) – the opened dataset as a cube.
```

Returns

Returns a string which describes the profile.

**Return type** 

str

```
esmvaltool.diag_scripts.ocean.diagnostic_profiles.main(cfg)
```

Run the diagnostics profile tool.

Load the config file, find an observational dataset filename, pass loaded into the plot making tool.

#### **Parameters**

**cfg** (*dict*) – the opened global config dictionairy, passed by ESMValTool.

esmvaltool.diag\_scripts.ocean.diagnostic\_profiles.make\_profiles\_plots(cfg, metadata, filename,

obs\_metadata={},
obs\_filename='')

Make a profile plot for an individual model.

The optional observational dataset can also be added.

## Parameters

- **cfg** (*dict*) the opened global config dictionairy, passed by ESMValTool.
- metadata (dict) The metadata dictionairy for a specific model.
- filename (str) The preprocessed model file.
- **obs\_metadata** (*dict*) The metadata dictionairy for the observational dataset.

• **obs\_filename** (*str*) – The preprocessed observational dataset file.

# 54.4.5 Time series diagnostics

Diagnostic to produce figures of the time development of a field from cubes. These plost show time on the x-axis and cube value (ie temperature) on the y-axis.

Two types of plots are produced: individual model timeseries plots and multi model time series plots. The inidivual plots show the results from a single cube, even if this is a multi-model mean made by the \_multimodel.py preproccessor. The multi model time series plots show several models on the same axes, where each model is represented by a different line colour.

Note that this diagnostic assumes that the preprocessors do the bulk of the hard work, and that the cube received by this diagnostic (via the settings.yml and metadata.yml files) has a time component, no depth component, and no latitude or longitude coordinates.

An approproate preprocessor for a 3D+time field would be:

```
preprocessors:
    prep_timeseries_1:# For Global Volume Averaged
    volume_statistics:
        operator: mean
```

An approproate preprocessor for a 3D+time field at the surface would be:

```
prep_timeseries_2: # For Global surface Averaged
extract_levels:
    levels: [0., ]
    scheme: linear_extrap
    area_statistics:
    operator: mean
```

An approproate preprocessor for a 2D+time field would be:

```
prep_timeseries_2: # For Global surface Averaged
area_statistics:
    operator: mean
```

This tool is part of the ocean diagnostic tools package in the ESMValTool.

## Author: Lee de Mora (PML)

ledm@pml.ac.uk

## **Functions:**

<pre>main(cfg)</pre>	Load the config file and some metadata, then pass them the plot making tools.
<pre>make_time_series_plots(cfg, metadata, filename)</pre>	Make a simple time series plot for an indivudual model 1D cube.
<pre>moving_average(cube, window)</pre>	Calculate a moving average.
<pre>multi_model_time_series(cfg, metadata)</pre>	Make a time series plot showing several preprocesssed datasets.
<pre>timeplot(cube, **kwargs)</pre>	Create a time series plot from the cube.

esmvaltool.diag\_scripts.ocean.diagnostic\_timeseries.main(cfg)

Load the config file and some metadata, then pass them the plot making tools.

## Parameters

cfg (dict) – the opened global config dictionairy, passed by ESMValTool.

```
esmvaltool.diag_scripts.ocean.diagnostic_timeseries.make_time_series_plots(cfg, metadata,
```

filename)

Make a simple time series plot for an indivudual model 1D cube.

This tool loads the cube from the file, checks that the units are sensible BGC units, checks for layers, adjusts the titles accordingly, determines the ultimate file name and format, then saves the image.

## Parameters

- **cfg** (*dict*) the opened global config dictionairy, passed by ESMValTool.
- **metadata** (*dict*) The metadata dictionairy for a specific model.
- **filename** (*str*) The preprocessed model file.

esmvaltool.diag\_scripts.ocean.diagnostic\_timeseries.moving\_average(cube, window)

Calculate a moving average.

The window is a string which is a number and a measuremet of time. For instance, the following are acceptable window strings:

- 5 days
- 12 years
- 1 month
- 5 yr

Also note the value used is the total width of the window. For instance, if the window provided was '10 years', the the moving average returned would be the average of all values within 5 years of the central value.

In the case of edge conditions, at the start an end of the data, they only include the average of the data available. Ie the first value in the moving average of a 10 year window will only include the average of the five subsequent years.

#### Parameters

- cube (iris.cube.Cube) Input cube
- window (str) A description of the window to use for the

#### Returns

A cube with the movinage average set as the data points.

#### **Return type**

iris.cube.Cube

esmvaltool.diag\_scripts.ocean.diagnostic\_timeseries.multi\_model\_time\_series(cfg, metadata)

Make a time series plot showing several preprocesssed datasets.

This tool loads several cubes from the files, checks that the units are sensible BGC units, checks for layers, adjusts the titles accordingly, determines the ultimate file name and format, then saves the image.

#### **Parameters**

- **cfg** (*dict*) the opened global config dictionairy, passed by ESMValTool.
- **metadata** (*dict*) The metadata dictionairy for a specific model.

esmvaltool.diag\_scripts.ocean.diagnostic\_timeseries.timeplot(cube, \*\*kwargs)

Create a time series plot from the cube.

Note that this function simple does the plotting, it does not save the image or do any of the complex work. This function also takes and of the key word arguments accepted by the matplotlib.pyplot.plot function. These arguments are typically, color, linewidth, linestyle, etc...

If there's only one datapoint in the cube, it is plotted as a horizontal line.

Parameters cube (iris.cube.Cube) – Input cube

## 54.4.6 Transects diagnostics

Diagnostic to produce images of a transect. These plost show either latitude or longitude against depth, and the cube value is used as the colour scale.

Note that this diagnostic assumes that the preprocessors do the bulk of the hard work, and that the cube received by this diagnostic (via the settings.yml and metadata.yml files) has no time component, and one of the latitude or longitude coordinates has been reduced to a single value.

An approproate preprocessor for a 3D+time field would be:

```
preprocessors:
    prep_transect:
        climate_statistics:
        operator: mean
        extract_transect: # Atlantic Meridional Transect
        latitude: [-50.,50.]
        longitude: 332.
```

This tool is part of the ocean diagnostic tools package in the ESMValTool.

## Author: Lee de Mora (PML)

ledm@pml.ac.uk

### **Functions:**

add_sea_floor(cube)	Add a simple sea floor line from the cube mask.
<pre>determine_set_y_logscale(cfg, metadata)</pre>	Determine whether to use a log scale y axis.
<pre>determine_transect_str(cube[, region])</pre>	Determine the Transect String.
<pre>main(cfg)</pre>	Load the config file and some metadata, then pass them the plot making tools.
<pre>make_cube_region_dict(cube)</pre>	Take a cube and return a dictionairy region: cube.
<pre>make_depth_safe(cube)</pre>	Make the depth coordinate safe.
<pre>make_transect_contours(cfg, metadata, filename)</pre>	Make a contour plot of the transect for an indivudual model.
<pre>make_transects_plots(cfg, metadata, filename)</pre>	Make a simple plot of the transect for an indivudual model.
<pre>multi_model_contours(cfg, metadatas)</pre>	Make a multi model comparison plot showing several transect contour plots.
titlify(title)	Check whether a title is too long then add it to current figure.

esmvaltool.diag\_scripts.ocean.diagnostic\_transects.add\_sea\_floor(cube)

Add a simple sea floor line from the cube mask.

#### **Parameters**

cube (iris.cube.Cube) – Input cube to use to produce the sea floor.

esmvaltool.diag\_scripts.ocean.diagnostic\_transects.determine\_set\_y\_logscale(*cfg*, *metadata*) Determine whether to use a log scale y axis.

#### **Parameters**

• **cfg** (*dict*) – the opened global config dictionairy, passed by ESMValTool.

• metadata (dict) – The metadata dictionairy for a specific model.

#### Returns

Boolean to flag whether to plot as a log scale.

## **Return type**

bool

esmvaltool.diag\_scripts.ocean.diagnostic\_transects.determine\_transect\_str(cube, region=")
Determine the Transect String.

Takes a guess at a string to describe the transect.

#### **Parameters**

cube (iris.cube.Cube) – Input cube to use to determine the transect name.

esmvaltool.diag\_scripts.ocean.diagnostic\_transects.main(cfg)

Load the config file and some metadata, then pass them the plot making tools.

#### **Parameters**

**cfg** (*dict*) – the opened global config dictionairy, passed by ESMValTool.

esmvaltool.diag\_scripts.ocean.diagnostic\_transects.make\_cube\_region\_dict(cube)

Take a cube and return a dictionairy region: cube.

Each item in the dict is a layer with a separate cube for each layer. ie: cubes[region] = cube from specific region

Cubes with no region component are returns as: cubes[''] = cube with no region component.

This is based on the method diagnostics\_tools.make\_cube\_layer\_dict, however, it wouldn't make sense to look for depth layers here.

#### Parameters

cube (iris.cube.Cube) – the opened dataset as a cube.

## Returns

A dictionairy of layer name : layer cube.

## **Return type**

dict

esmvaltool.diag\_scripts.ocean.diagnostic\_transects.make\_depth\_safe(cube)

Make the depth coordinate safe.

If the depth coordinate has a value of zero or above, we replace the zero with the average point of the first depth layer.

## Parameters

cube (iris.cube.Cube) - Input cube to make the depth coordinate safe

### Returns

Output cube with a safe depth coordinate

#### **Return type**

iris.cube.Cube

```
esmvaltool.diag_scripts.ocean.diagnostic_transects.make_transect_contours(cfg, metadata,
```

filename)

Make a contour plot of the transect for an indivudual model.

This tool loads the cube from the file, checks that the units are sensible BGC units, checks for layers, adjusts the titles accordingly, determines the ultimate file name and format, then saves the image.

## Parameters

- **cfg** (*dict*) the opened global config dictionairy, passed by ESMValTool.
- **metadata** (*dict*) The metadata dictionairy for a specific model.
- **filename** (*str*) The preprocessed model file.

Make a simple plot of the transect for an indivudual model.

This tool loads the cube from the file, checks that the units are sensible BGC units, checks for layers, adjusts the titles accordingly, determines the ultimate file name and format, then saves the image.

## Parameters

- **cfg** (*dict*) the opened global config dictionairy, passed by ESMValTool.
- **metadata** (*dict*) The metadata dictionairy for a specific model.
- **filename** (*str*) The preprocessed model file.

esmvaltool.diag\_scripts.ocean.diagnostic\_transects.multi\_model\_contours(cfg, metadatas)

Make a multi model comparison plot showing several transect contour plots.

This tool loads several cubes from the files, checks that the units are sensible BGC units, checks for layers, adjusts the titles accordingly, determines the ultimate file name and format, then saves the image.

## Parameters

- **cfg** (*dict*) the opened global config dictionairy, passed by ESMValTool.
- metadatas (dict) The metadatas dictionairy for a specific model.

esmvaltool.diag\_scripts.ocean.diagnostic\_transects.titlify(title)

Check whether a title is too long then add it to current figure.

## Parameters

**title** (*str*) – The title for the figure.

# 54.4.7 Sea Ice Diagnostics.

Diagnostic to produce a series of images which are useful for evaluating the behaviour of the a sea ice model.

There are three kinds of plots shown here. 1. Sea ice Extent maps plots with a stereoscoic projection. 2. Maps plots of individual models ice fraction. 3. Time series plots for the total ice extent.

All three kinds of plots are made for both Summer and Winter in both the North and Southern hemisphere.

Note that this diagnostic assumes that the preprocessors do the bulk of the hard work, and that the cube received by this diagnostic (via the settings.yml and metadata.yml files) has no time component, a small number of depth layers, and a latitude and longitude coordinates.

This diagnostic takes data from either North or South hemisphere, and from either December-January-February or June-July-August. This diagnostic requires the data to be 2D+time, and typically expects the data field to be the sea ice cover. An appropriate preprocessor would be:

```
preprocessors:
  timeseries_NHW_ice_extent: # North Hemisphere Winter ice_extent
    custom_order: true
    extract_time:
        start_year: 1960
        start_month: 12
        start_day: 1
        end_year: 2005
        end_month: 9
        end_day: 31
    extract_season:
      season: DJF
    extract_region:
      start_longitude: -180.
      end_longitude: 180.
      start_latitude: 0.
      end latitude: 90.
```

Note that this recipe may not function on machines with no access to the internet, as cartopy may try to download the shapefiles. The solution to this issue is the put the relevant cartopy shapefiles on a disk visible to your machine, then link that path to ESMValTool via the *auxiliary\_data\_dir* variable. The cartopy masking files can be downloaded from:

https://www.naturalearthdata.com/downloads/

Here, cartopy uses the 1:10, physical coastlines and land files:

```
110m_coastline.dbf 110m_coastline.shp 110m_coastline.shx
110m_land.dbf 110m_land.shp 110m_land.shx
```

This tool is part of the ocean diagnostic tools package in the ESMValTool.

```
Author: Lee de Mora (PML)
ledm@pml.ac.uk
```

**Functions:** 

<pre>agregate_by_season(cube)</pre>	Aggregate the cube into seasonal means.
<pre>calculate_area_time_series(cube, plot_type,)</pre>	Calculate the area of unmasked cube cells.
<pre>create_ice_cmap([threshold])</pre>	Create colour map with ocean blue below a threshold and white above.
<pre>get_pole(cube)</pre>	Figure out the hemisphere and returns it as a string (North or South).
<pre>get_season(cube)</pre>	Return a climatological season time string.
<pre>get_time_string(cube)</pre>	Return a climatological season string in the format: "year season".
<pre>get_year(cube)</pre>	Return the cube year as a string.
main(cfg)	Load the config file and metadata, then pass them the plot making tools.
<pre>make_map_extent_plots(cfg, metadata, filename)</pre>	Make an extent map plot showing several times for an individual model.
<pre>make_map_plots(cfg, metadata, filename)</pre>	Make a simple map plot for an individual model.
<pre>make_polar_map(cube[, pole, cmap])</pre>	Make a polar stereoscopic map plot.
<pre>make_ts_plots(cfg, metadata, filename)</pre>	Make a ice extent and ice area time series plot for an individual model.

### esmvaltool.diag\_scripts.ocean.diagnostic\_seaice.agregate\_by\_season(cube)

Aggregate the cube into seasonal means.

Note that it is not currently possible to do this in the preprocessor, as the seasonal mean changes the cube units.

# Parameters cube (iris.cube.Cube) – Data Cube

# Returns

Data Cube with the seasonal means

### **Return type**

iris.cube.Cube

esmvaltool.diag\_scripts.ocean.diagnostic\_seaice.calculate\_area\_time\_series(cube, plot\_type,

threshold)

Calculate the area of unmasked cube cells.

Requires a cube with two spacial dimensions. (no depth coordinate).

Parameters

- cube (iris.cube.Cube) Data Cube
- **plot\_type** (*str*) The type of plot: ice extent or ice area
- **threshold** (*float*) The threshold for ice fraction (typically 15%)

# Returns

- *numpy array* An numpy array containing the time points.
- numpy.array An numpy array containing the total ice extent or total ice area.

esmvaltool.diag\_scripts.ocean.diagnostic\_seaice.create\_ice\_cmap(threshold=0.15)

Create colour map with ocean blue below a threshold and white above.

### **Parameters**

threshold (float) – The threshold for the line between blue and white.

### Returns

The resulting colour map.

### **Return type**

matplotlib.colors.LinearSegmentedColormap

esmvaltool.diag\_scripts.ocean.diagnostic\_seaice.get\_pole(cube)

Figure out the hemisphere and returns it as a string (North or South).

### **Parameters**

cube (iris.cube.Cube) – Data Cube

### Returns

The hemisphere (North or South)

# **Return type**

str

esmvaltool.diag\_scripts.ocean.diagnostic\_seaice.get\_season(cube)

Return a climatological season time string.

### Parameters

cube (iris.cube.Cube) – Data Cube

# Returns

The climatological season as a string

### **Return type**

str

```
esmvaltool.diag_scripts.ocean.diagnostic_seaice.get_time_string(cube)
```

Return a climatological season string in the format: "year season".

# Parameters

cube (iris.cube.Cube) – Data Cube

# Returns

The climatological season as a string

### **Return type**

str

esmvaltool.diag\_scripts.ocean.diagnostic\_seaice.get\_year(cube)

Return the cube year as a string.

# Parameters

cube (iris.cube.Cube) – Data Cube

# Returns

The year as a string

# **Return type**

str

# esmvaltool.diag\_scripts.ocean.diagnostic\_seaice.main(cfg)

Load the config file and metadata, then pass them the plot making tools.

# **Parameters**

cfg (dict) – the opened global config dictionairy, passed by ESMValTool.

esmvaltool.diag\_scripts.ocean.diagnostic\_seaice.make\_map\_extent\_plots(cfg, metadata, filename)
Make an extent map plot showing several times for an individual model.

# Parameters

- **cfg** (*dict*) the opened global config dictionairy, passed by ESMValTool.
- **metadata** (*dict*) The metadata dictionairy for a specific model.
- filename (str) The preprocessed model file.

esmvaltool.diag\_scripts.ocean.diagnostic\_seaice.make\_map\_plots(cfg, metadata, filename)
Make a simple map plot for an individual model.

# Parameters

- **cfg** (*dict*) the opened global config dictionairy, passed by ESMValTool.
- **metadata** (*dict*) The metadata dictionairy for a specific model.
- filename (str) The preprocessed model file.

Make a polar stereoscopic map plot.

The cube is the opened cube (two dimensional), pole is the polar region (North/South) cmap is the colourmap,

# **Parameters**

- cube (iris.cube.Cube) Data Cube
- **pole** (*str*) The hemisphere
- **cmap** (*str*) The string describing the matplotlib colourmap.

# Returns

- *matplotlib.pyplot.figure* The matplotlib figure where the map was drawn.
- *matplotlib.pyplot.axes* The matplotlib axes where the map was drawn.

esmvaltool.diag\_scripts.ocean.diagnostic\_seaice.make\_ts\_plots(cfg, metadata, filename)

Make a ice extent and ice area time series plot for an individual model.

# Parameters

- **cfg** (*dict*) the opened global config dictionairy, passed by ESMValTool.
- metadata (dict) The metadata dictionairy for a specific model.
- filename (str) The preprocessed model file.

# 54.4.8 Diagnostic tools

This module contains several python tools used elsewhere by the ocean diagnostics package.

This tool is part of the ocean diagnostic tools package in the ESMValTool.

Author: Lee de Mora (PML)

ledm@pml.ac.uk

# **Functions:**

<pre>add_legend_outside_right(plot_details, ax1)</pre>	Add a legend outside the plot, to the right.
<i>bgc_units</i> (cube, name)	Convert the cubes into some friendlier units.
<pre>cube_time_to_float(cube)</pre>	Convert from time coordinate into decimal time.
decadal_average(cube)	Calculate the decadal_average.
folder(name)	Make a directory out of a string or list or strings.
get_array_range(arrays)	Determinue the minimum and maximum values of a list of arrays
<pre>get_colour_from_cmap(number, total[, cmap])</pre>	Get a colour <i>number</i> of <i>total</i> from a cmap.
<pre>get_cube_range(cubes)</pre>	Determinue the minimum and maximum values of a list of cubes.
<pre>get_cube_range_diff(cubes)</pre>	Determinue the largest deviation from zero in an list of cubes.
<pre>get_decade(coord, value)</pre>	Determine the decade.
<pre>get_image_format(cfg[, default])</pre>	Load the image format from the global config file.
<pre>get_image_path(cfg, metadata[, prefix,])</pre>	Produce a path to the final location of the image.
<pre>get_input_files(cfg[, index])</pre>	Load input configuration file as a Dictionairy.
<pre>get_obs_projects()</pre>	Return a list of strings with the names of observations projects.
<pre>guess_calendar_datetime(cube)</pre>	Guess the cftime.datetime form to create datetimes.
<i>load_thresholds</i> (cfg, metadata)	Load the thresholds for contour plots from the config files.
<pre>make_cube_layer_dict(cube)</pre>	Take a cube and return a dictionary layer:cube
<pre>match_model_to_key(model_type, cfg_dict,)</pre>	Match up model or observations dataset dictionairies from config file.
prepare_provenance_record(cfg,)	Prepare informations to feed provenance

Add a legend outside the plot, to the right.

plot\_details is a 2 level dict, where the first level is some key (which is hidden) and the 2nd level contains the keys: 'c': color 'lw': line width 'label': label for the legend. ax1 is the axis where the plot was drawn.

# Parameters

- plot\_details (dict) A dictionary of the plot details (color, linestyle, linewidth, label)
- **ax1** (*matplotlib.pyplot.axes*) The pyplot axes to add the
- **column\_width** (*float*) The width of the legend column. This is used to adjust for longer words in the legends
- loc (string) Location of the legend. Options are "right" and "below".

### Returns

A datetime creator function from cftime, based on the cube's calendar.

# **Return type**

cftime.datetime

esmvaltool.diag\_scripts.ocean.diagnostic\_tools.bgc\_units(cube, name)

Convert the cubes into some friendlier units.

This is because many CMIP standard units are not the standard units used by the BGC community (ie, Celsius is prefered over Kelvin, etc.)

# **Parameters**

- cube (iris.cube.Cube) the opened dataset as a cube.
- **name** (*str*) The string describing the data field.

# Returns

the cube with the new units.

### Return type

iris.cube.Cube

# esmvaltool.diag\_scripts.ocean.diagnostic\_tools.cube\_time\_to\_float(cube)

Convert from time coordinate into decimal time.

Takes an iris time coordinate and returns a list of floats. :param cube: the opened dataset as a cube. :type cube: iris.cube.Cube

#### Returns

List of floats showing the time coordinate in decimal time.

### Return type list

esmvaltool.diag\_scripts.ocean.diagnostic\_tools.decadal\_average(cube)

Calculate the decadal\_average.

Parameters cube (*iris.cube.Cube*) – The input cube Return type

iris.cube

esmvaltool.diag\_scripts.ocean.diagnostic\_tools.folder(name)

Make a directory out of a string or list or strings.

Take a string or a list of strings, convert it to a directory style, then make the folder and the string. Returns folder string and final character is always os.sep. ('/')

### Parameters

**name** (*list or string*) – A list of nested directories, or a path to a directory.

### Returns

Returns a string of a full (potentially new) path of the directory.

#### Return type

str

esmvaltool.diag\_scripts.ocean.diagnostic\_tools.get\_array\_range(arrays)

Determinue the minimum and maximum values of a list of arrays..

### Parameters

arrays (list of numpy.array) – A list of numpy.array.

#### Returns

A list of two values, the overall minumum and maximum values of the list of cubes.

### **Return type**

list

esmvaltool.diag\_scripts.ocean.diagnostic\_tools.get\_colour\_from\_cmap(number, total, cmap='jet') Get a colour number of total from a cmap.

This function is used when several lines are created evenly along a colour map.

### **Parameters**

- number (int, float) The
- total (int)
- cmap (string, plt.cm) A colour map, either by name (string) or from matplotlib

esmvaltool.diag\_scripts.ocean.diagnostic\_tools.get\_cube\_range(cubes)

Determinue the minimum and maximum values of a list of cubes.

#### Parameters

cubes (list of iris.cube.Cube) - A list of cubes.

#### Returns

A list of two values: the overall minumum and maximum values of the list of cubes.

#### **Return type**

list

esmvaltool.diag\_scripts.ocean.diagnostic\_tools.get\_cube\_range\_diff(cubes)

Determinue the largest deviation from zero in an list of cubes.

### **Parameters**

cubes (list of iris.cube.Cube) – A list of cubes.

### Returns

A list of two values: the maximum deviation from zero and its opposite.

### **Return type**

list

esmvaltool.diag\_scripts.ocean.diagnostic\_tools.get\_decade(coord, value)

Determine the decade.

Called by iris.coord\_categorisation.add\_categorised\_coord.

```
esmvaltool.diag_scripts.ocean.diagnostic_tools.get_image_format(cfg, default='png')
```

Load the image format from the global config file.

Current tested options are svg, png.

The cfg is the opened global config. The default format is used if no specific format is requested. The default is set in the user config.yml Individual diagnostics can set their own format which will supercede the main config.yml.

### Parameters

**cfg** (*dict*) – the opened global config dictionary, passed by ESMValTool.

#### Returns

The image format extention.

#### **Return type**

str

Produce a path to the final location of the image.

The cfg is the opened global config, metadata is the metadata dictionary (for the individual dataset file)

# Parameters

• **cfg** (*dict*) – the opened global config dictionary, passed by ESMValTool.

- metadata (dict) The metadata dictionary for a specific model.
- **prefix** (*str*) A string to prepend to the image basename.
- **suffix** (*str*) A string to append to the image basename
- **metadata\_id\_list** (*list*) A list of strings to add to the file path. It loads these from the cfg.

## Returns

The ultimate image path

#### **Return type**

str

esmvaltool.diag\_scripts.ocean.diagnostic\_tools.get\_input\_files(cfg, index=")

Load input configuration file as a Dictionairy.

Get a dictionary with input files from the metadata.yml files. This is a wrappper for the \_get\_input\_data\_files function from diag\_scripts.shared.\_base.

# **Parameters**

- **cfg** (*dict*) the opened global config dictionary, passed by ESMValTool.
- **index** (*int*) the index of the file in the cfg file.

### Returns

A dictionary of the input files and their linked details.

# **Return type**

dict

```
esmvaltool.diag_scripts.ocean.diagnostic_tools.get_obs_projects()
```

Return a list of strings with the names of observations projects.

Please keep this list up to date, or replace it with something more sensible.

### Returns

Returns a list of strings of the various types of observational data.

#### **Return type**

list

```
esmvaltool.diag_scripts.ocean.diagnostic_tools.guess_calendar_datetime(cube)
```

Guess the cftime.datetime form to create datetimes.

# Parameters

cube (iris.cube.Cube) – the opened dataset as a cube.

# Returns

A datetime creator function from cftime, based on the cube's calendar.

### **Return type**

cftime.datetime

esmvaltool.diag\_scripts.ocean.diagnostic\_tools.load\_thresholds(*cfg*, *metadata*) Load the thresholds for contour plots from the config files.

### **Parameters**

- **cfg** (*dict*) the opened global config dictionary, passed by ESMValTool.
- metadata (dict) the metadata dictionary

#### Returns

List of thresholds

# **Return type**

list

esmvaltool.diag\_scripts.ocean.diagnostic\_tools.make\_cube\_layer\_dict(cube)

Take a cube and return a dictionary layer:cube

Each item in the dict is a layer with a separate cube for each layer. ie: cubes[depth] = cube from specific layer

Cubes with no depth component are returned as dict, where the dict key is a blank empty string, and the value is the cube.

# **Parameters**

cube (iris.cube.Cube) – the opened dataset as a cube.

### Returns

A dictionary of layer name : layer cube.

Return type

Match up model or observations dataset dictionairies from config file.

This function checks that the control\_model, exper\_model and observational\_dataset dictionairies from the recipe are matched with the input file dictionary in the cfg metadata.

### **Parameters**

- **model\_type** (*str*) The string model\_type to match (only used in debugging).
- **cfg\_dict** (*dict*) the config dictionary item for this model type, parsed directly from the diagnostics/ scripts, part of the recipe.
- input\_files\_dict (dict) -
  - **The input file dictionary, loaded directly from the get\_input\_files**() function, in diagnostics\_tools.py.

### Returns

A dictionary of the input files and their linked details.

# **Return type**

dict

esmvaltool.diag\_scripts.ocean.diagnostic\_tools.prepare\_provenance\_record(cfg, \*\*provenance\_record)

Prepare informations to feed provenance

# **Parameters**

- **cfg** (*dict*) the opened global config dictionary, passed by ESMValTool.
- **provenance\_record** (*dict*) dictionary for a specific diagnostic provenance details.

# 54.5 Psyplot Diagnostic

Create arbitrary Psyplot plots.

# 54.5.1 Description

This diagnostic provides a high-level interface to Psyplot.

# 54.5.2 Author

Manuel Schlund (DLR, Germany)

# Notes

For each input dataset, an individual plot is created. This diagnostic supports arbitrary variables of arbitrary datasets.

# 54.5.3 Configuration options in recipe

# psyplot\_func: str

Function used to plot the data. Must be a function of psyplot.project.plot. Run python -c "from psyplot.project import plot; print(plot.show\_plot\_methods())" to get a list of all currently supported plotting functions (make sure to run this command in your ESMValTool environment).

# psyplot\_kwargs: dict, optional

Optional keyword arguments for the plotting function given by psyplot\_func. String arguments can include facets in curly brackets which will be derived from the corresponding dataset, e.g., clabel: '{long\_name} [{units}]', title: '{long\_name} Climatology of {dataset} ({start\_year}-{end\_year})'.

# savefig\_kwargs: dict, optional

Optional keyword arguments for matplotlib.pyplot.savefig(). By default, uses bbox\_inches: tight, dpi: 300, orientation: landscape.

# seaborn\_settings: dict, optional

Options for seaborn.set\_theme() (affects all plots).

# 54.6 Seaborn Diagnostic

Create arbitrary Seaborn plots.

# 54.6.1 Description

This diagnostic provides a high-level interface to Seaborn. For this, the input data is arranged into a single pandas. DataFrame, which is then used as input for the Seaborn function defined by the option *seaborn\_func*.

# 54.6.2 Caveats

All datasets of a given variable must have the same units (e.g., it is not allowed to use datasets with units K and datasets with units  $^{\circ}C$  for the variable *tas*).

# 54.6.3 Author

Manuel Schlund (DLR, Germany)

# 54.6.4 Configuration options in recipe

# add\_ancillary\_variables: bool, optional (default: False)

Add ancillary\_variables() to the main data frame. Note that this will assume that ancillary variables are identical across cubes within a group (see option *groupby\_facet*). This equality is not checked!

# add\_aux\_coords: bool, optional (default: False)

Add aux\_coords to the main data frame. Note that this will assume that auxiliary coordinates are identical across cubes within a group (see option *groupby\_facet*). This equality is not checked!

# add\_cell\_measures: bool, optional (default: False)

Add cell\_measures() to the main data frame. Note that this will assume that cell measures are identical across cubes within a group (see option *groupby\_facet*). This equality is not checked!

# data\_frame\_ops: dict, optional

Perform additional operations on the main data frame. Allowed operations are pandas.DataFrame.query() (dict key *query*) and pandas.DataFrame.eval() (dict key *eval*). Operations are defined by strings (dict values). Examples: {'query': 'latitude > 80', 'eval': 'longitude = longitude - 180.0'}.

# dropna\_kwargs: dict, optional

Optional keyword arguments for pandas.DataFrame.dropna() to drop missing values in the input data. If not given, do not drop NaNs. Note: NaNs are dropped after potential *data\_frame\_ops*.

# facets\_as\_columns: list of str, optional

Facets that will be added as a columns to the main data frame. Values for these facets must be identical across all datasets within a group (see option *groupby\_facet*).

# groupby\_facet: str, optional (default: 'alias')

Facet which is used to group input datasets when creating the main data frame. All datasets within a group are expected to have the same index after calling iris.pandas.as\_data\_frame() on them. These datasets within a group will then get merged (combined along axis 1, i.e., columns) into a single data frame per group. Finally, the data frames for all groups are concatenated (combined along axis 0, i.e., rows) into one main data frame. *groupby\_facet* is also added as a column to this main data frame.

# legend\_title: str, optional (default: None)

Title for legend. If None, Seaborn will determine the legend title (if possible).

# plot\_object\_methods: dict, optional

Execute methods of the object returned by the plotting function (*seaborn\_func*). This object will either be a matplotlib.axes.Axes (e.g., scatterplot(), lineplot()), a seaborn.FacetGrid (e.g., relplot(), displot()), a seaborn.JointGrid (e.g., jointplot()), or a seaborn.PairGrid (e.g., pairplot()). Dictionary keys are method names, dictionary values function arguments (use a dict to specify keyword arguments). Example (for relplot()): {'set': {'xlabel': 'X [km]'}, 'set\_titles': 'Model {col\_name}'}.

# reset\_index: bool, optional (default: False)

Put coordinate information of datasets into columns instead of (multi-) indices. This avoids the deletion of coordinate information if different groups of datasets have different dimensions but increases the memory footprint of this diagnostic.

# savefig\_kwargs: dict, optional

Optional keyword arguments for matplotlib.pyplot.savefig(). By default, uses bbox\_inches: tight, dpi: 300, orientation: landscape.

# seaborn\_func: str

Function used to plot the data. Must be a function of Seaborn. An overview of Seaborn's plotting functions is given here.

### seaborn\_kwargs: dict, optional

Optional keyword arguments for the plotting function given by *seaborn\_func*. Must not include an argument called *data*. Example: {'x': 'variable\_1', 'y': 'variable\_2', 'hue': 'coord\_1'}. Note: variables (here: *variable\_1* and *variable\_2* are identified by their *variable\_group* in the recipe, i.e., the keys that specify variable groups in *variables*.

# seaborn\_settings: dict, optional

Options for seaborn.set\_theme() (affects all plots).

# suptitle: str or None, optional (default: None)

Suptitle for the plot (see matplotlib.pyplot.suptitle()). If None, do not create a suptitle. If the plot shows only a single panel, use *plot\_object\_methods* with {'set': {'title': 'TITLE'}} instead.

# Part XI

# **Frequently Asked Questions**

# FIFTYFIVE

# **IS THERE A MAILING LIST?**

Yes, you can subscribe to the ESMValTool user mailing list and join the discussion on general topics (installation, configuration, etc). See *User mailing list*.

# **FIFTYSIX**

# WHAT IS YAML?

While .yaml or .yml is a relatively common format, users may not have encountered this language before. The key information about this format is:

- yaml is a human friendly markup language;
- yaml is commonly used for configuration files (gradually replacing the venerable .ini);
- the syntax is relatively straightforward;
- indentation matters a lot (like Python)!
- yaml is case sensitive;

More information can be found in the yaml tutorial and yaml quick reference card. ESMValTool uses the yamllint linter tool to check recipe syntax.

# **FIFTYSEVEN**

# **RE-RUNNING DIAGNOSTICS**

If a diagnostic fails, you will get the message

INFO To re-run this diagnostic script, run:

If you run the command in the stdout you will be able to re-run the diagnostic without having to re-run the whole preprocessor. If you add the -f argument (available only for Python diagnostics, check your options with --help) that will force an overwrite, and it will delete not just the failed diagnostic, but the contents of its work\_dir and plot\_dir directories - this is useful when needing to redo the whole work. Adding -i or --ignore-existing will not delete any existing files, and it can be used to skip work that was already done successfully, provided that the diagnostic script supports this.

# FIFTYEIGHT

# ENTER INTERACTIVE MODE WITH IPYTHON

Sometimes it is useful to enter an interactive session to have a look what's going on. Insert a single line in the code where you want to enter IPython: import IPython; IPython.embed()

This is a useful functionality because it allows the user to *fix* things on-the-fly and after quitting the Ipython console, code execution continues as per normal.

# FIFTYNINE

# **USE MULTIPLE CONFIG-USER.YML FILES**

The user selects the configuration yaml file at run time. It's possible to have several configurations files. For instance, it may be practical to have one config file for debugging runs and another for production runs.

SIXTY

# **CREATE A SYMBOLIC LINK TO THE LATEST OUTPUT DIRECTORY**

When running multiple times the same recipe, the tool creates separate output directories sorted by the time tag that they were created at; sometimes, when running quite a few times, it is not straightforward to detect which one is the *latest* output directory, so a symbolic link attached to it would make things more clear e.g.:

```
recipe_example_20190905_163431
recipe_example_20190905_163519
recipe_example_latest -> recipe_example_20190905_163519
```

You can do that by running the tool using the latest output as basis and creating a symbolic link to it so it gets picked up at every re-run iteration:

# SIXTYONE

# CAN ESMVALTOOL PLOT ARBITRARY MODEL OUTPUT?

*General model evaluation* provides a set of recipes that can be used for a basic climate model evaluation with observational data. This is especially useful to get an overview of the general performance of a simulation.

Furthermore, recipe *Monitor* allows for the plotting of any preprocessed model. The plotting parameters are set through a yaml configuration file, and the type of plots to be generated are determined in the recipe.

Moreover, recipe *Psyplot Diagnostics* and the corresponding diagnostic *psyplot\_diag.py* provide a high-level interface to the Psyplot package which can be used to create a large variety of different plots.

Similarly, recipe *Seaborn Diagnostics* and the corresponding diagnostic *seaborn\_diag.py* provide a high-level interface to the Seaborn package which can also be used to create a large variety of different plots.

See also General-purpose diagnostics.

# Part XII

# Changelog

# SIXTYTWO

# V2.10.0

# Highlights

- Add a realistic IPCC example recipe that reproduces figure 9.3 from AR6. It computes the mean sea-surface temperature anomaly between 1850-2100 over all available CMIP6 models. See the *recipe documentation* or read the blog post for more information.
- Added more plot types to monitoring diagnostic: Hovmoeller Z vs. time, Hovmoeller time vs latlon, variable vs. latitude are now available. See the *recipe documentation* for more information.
- Add support for 4 new datasets:
  - NOAA-CIRES-20CR v3 reanalysis
  - NASA MERRA reanalysis
  - NOAA marine boundary layer data for CH4
  - MOBO-DIC2004-2019

See Supported datasets for which a CMORizer script is available and Observations for more information.

• Many recipes now have up-to-date obs4MIPs dataset names so required data can automatically be downloaded from ESGF.

This release includes

# 62.1 Bug fixes

- Update recipe shapeselect to work with shapely v2 (Pull request #3283) @lukruh
- Correctly handle ~ when reading plot\_folder option of monitoring diagnostic (Pull request #3449) @schlunma
- Fixed provenance tracking for NCL multipanel PNGs (Pull request #3332) @schlunma
- Fixed plot paths in NCL provenance tracking (Pull request #3422) @schlunma
- Fix erroneous file\_type handling in certain NCL diagnostics (Pull request #3474) @zklaus
- Fix NCL provenance tracking (Pull request #3477) @schlunma
- Fix plots and provenance in Russell diagnostics (Pull request #3479) @schlunma

# 62.2 Documentation

- Add merge instructions to release instructions (Pull request #3292) @remi-kazeroni
- Update release schedule after release of v2.9.0 (Pull request #3289) @remi-kazeroni
- Add list of failing recipes for v2.9.0 release (Pull request #3294) @remi-kazeroni
- Update mamba version in readthedocs configuration docs builds (Pull request #3310) @valeriupredoi
- Add Romain Beucher to citation file as contributor (Pull request #3318) @valeriupredoi
- Removed recipe\_carvalhais14nat from list of broken recipes (Pull request #3319) @remi-kazeroni
- Add OBS-maintainers team to documentation on OBS data maintenance and CMORizer reviews (Pull request #3335) @remi-kazeroni
- Add Pauline Bonnet to citation file (Pull request #3347) @Paulinebonnet111
- Ensure compatible zstandard and zstd in readthedocs builds (Pull request #3362) @zklaus
- Fix documentation build (Pull request #3397) @bouweandela
- Minor updates to release tools (Pull request #3216) @bouweandela
- Enhance provenance documentation (Pull request #3305) @alistairsellar
- Re-add communities and grants in zenodo file (Pull request #3416) @valeriupredoi
- Update Anconda badge in README (Pull request #3375, Pull request #3453) @valeriupredoi

# 62.3 Diagnostics

- Slight refactoring of diagnostic script galytska23/select\_variables\_for\_tigramite.py for generality and portability (Pull request #3298) @valeriupredoi and @egalytska
- Allow custom variable grouping in diagnostic script monitor/multi\_datasets.py (Pull request #3343) @schlunma
- Extended monitor diagnostic with plot type variable vs. latitude (Pull request #3340) @ellensarauer
- Add Hovmoeller Z vs. time plot to monitoring diagnostic (Pull request #3345) @cubeme and @helgehr
- Adding Hovmoeller time vs latlon plots to monitoring recipes (Pull request #3341) @lukruh and @jeremykraftdlr
- Implied heat transport new diagnostic (Pull request #3177) @mo-abodas
- Recipe changes for new statistics preprocessors (percentiles) (Pull request #3351) @schlunma
- Add a realistic example recipe (Pull request #3356) @Peter9191 and @bouweandela
- Support CenteredNorm in diagnostic monitor/multidatasets.py (Pull request #3415) @schlunma
- Use new preprocessor statistics calling convention for recipe\_easy\_ipcc.yml (Pull request #3418) @bouweandela
- Adapt to changed style scheme name in matplotlib (Pull request #3475) @zklaus
- Add version to dataset in python example recipe to avoid "Unknown file format" issue on JASMIN (Pull request #3322) @ehogan
- Add the dataset version in the heatwaves\_coldwaves recipe to avoid the "Unknown file format" issue on JASMIN (Pull request #3373) @ehogan

# 62.4 Observational and re-analysis dataset support

- Cmorizer for NOAA-CIRES-20CR v3 reanalysis (clt, clwvi, hus, prw, rlut, rlutcs, rsut, rsutcs) (Pull request #3137) @LisaBock
- CMORizer for NASA MERRA reanalysis (Pull request #3039) @axel-lauer
- Download and formatting of NOAA marine boundary layer data for CH4 (NOAA-MBL-CH4) (Pull request #3301) @FranziskaWinterstein
- Added CMORizer for MOBO-DIC2004-2019 (Pull request #3297) @schlunma
- Update obs4MIPs dataset names in quantilebias recipe (Pull request #3330) @rbeucher
- Update obs4MIPs dataset names in Schlund20esd recipe (Pull request #3329) @rbeucher
- Update obs4MIPs dataset names in flatoipcc recipes (Pull request #3328) @rbeucher
- Update obs4mips dataset names in clouds recipes (Pull request #3326) @rbeucher
- Update Obs4MIPs dataset names in ECS recipes (Pull request #3327) @rbeucher
- Update obs4mips dataset names in Bock et al recipes (Pull request #3324, Pull request #3389 and Pull request #3473) @rbeucher and @bouweandela
- Update obs4mips dataset names in radiation budget recipe (Pull request #3323) @rbeucher
- Update Obs4MIPs dataset names in perfmetrics CMIP5 recipe (Pull request #3325) @rbeucher

# 62.5 Automatic testing

- Made sklearn test backwards-compatible with sklearn < 1.3 (Pull request #3285) @schlunma
- Update conda lock creation Github Action workflow and ship updated conda-lock file (Pull request #3307, Pull request #3407) @valeriupredoi
- Compress all bash shell setters into one default option per GitHub Action workflow (Pull request #3315) @valeriupredoi
- Remove deprecated option offline from CI configuration (Pull request #3367) @schlunma

# 62.6 Installation

• Use ESMValCore v2.10 (Pull request #3486) @bouweandela

# 62.7 Improvements

- Merge v2.9.x into main (Pull request #3286) @schlunma
- Allow NCL unit conversion kg s-1 -> GtC y-1 (Pull request #3300) @schlunma

# SIXTYTHREE

# V2.9.0

# **63.1 Highlights**

- A new *diagnostic* has been added to provide a high-level interface to seaborn, a Python data visualization library based on matplotlib. See the *recipe documentation* for more information.
- We have included a new recipe and diagnostic that represent the major physical processes that describe Arcticmidlatitude teleconnections and provide the basis for the CMIP6 model evaluation for the further application of causal discovery. The results are discussed in the article "Causal model evaluation of Arctic-midlatitude teleconnections in CMIP6" by Galytska et al. (in review in Journal of Geophysical Research: Atmospheres).
- It is now possible to use the Dask distributed scheduler, which can significantly reduce the run-time of recipes. Configuration examples and advice are available in the ESMValCore documentation. If configured, the Dask distributed scheduler will also be used by diagnostic scripts written in Python, so make sure to use lazy data wherever it is possible in your (new) diagnostics. More work on improving the computational performance is planned, so please share your experiences, good and bad, with this new feature in ESMValGroup/ESMValCore#1763.

This release includes

# 63.2 Bug fixes

- Fixed usage of work\_dir in some CMORizer scripts (Pull request #3192) @remi-kazeroni
- Realize data for scalar cube in *recipe\_carvalhais14nat* to avert issue from dask latest (2023.6.0) (Pull request #3265) @valeriupredoi
- Fix failing mlr diagnostic test by adding new scikit-learn default tag (Pull request #3273) @remi-kazeroni
- Fix ordering of models in perfmetrics diagnostic script (Pull request #3275) @LisaBock

# 63.3 Documentation

- Update release schedule after v2.8.0 (Pull request #3138) @remi-kazeroni
- Added reference entry for Winterstein (Pull request #3154) @FranziskaWinterstein
- Show logo on PyPI (Pull request #3185) @valeriupredoi
- Add Release Managers for v2.9.0 and v2.10.0 (Pull request #3184) @remi-kazeroni
- Fix readthedocs build with esmpy>=8.4.0 and missing ESMFMKFILE variable (Pull request #3205) @valeri-upredoi

- Add ESMValCore release v2.8.1 into the documentation (Pull request #3235) @remi-kazeroni
- Modified links to the tutorial (Pull request #3236) @remi-kazeroni
- Fix gitter badge in README (Pull request #3258) @remi-kazeroni
- Add release notes for v2.9.0 (Pull request #3266) @bouweandela

# **63.4 Diagnostics**

- New plot\_type 1d\_profile in monitor (Pull request #3178) @FranziskaWinterstein
- Add Seaborn diagnostic (Pull request #3155) @schlunma
- New recipe and diagnostic for Arctic-midlatitude research (Pull request #3021) @egalytska
- Generate climatology on the fly for AutoAssess soil moisture (Pull request #3197) @alistairsellar
- Remove "fx\_variables" from recipe\_tebaldi21esd.yml (Pull request #3211) @hb326
- Remove "fx\_variables" from ipccwg1ar5ch9 recipes (Pull request #3215) @katjaweigel
- Remove "fx\_variables" from recipe\_wenzel14jgr.yml (Pull request #3212) @hb326
- Update obs4MIPs dataset to the current naming scheme in recipe\_smpi.yml (Pull request #2991) @bouweandela
- Fixed pandas diagnostics for pandas>=2.0.0 (Pull request #3209) @schlunma
- Update recipe\_impact.yml to work with newer versions of pandas (Pull request #3220) @bouweandela
- Add variable long names to provenance record in monitoring diagnostics (Pull request #3222) @bsolino

# 63.5 Observational and re-analysis dataset support

- Add CMORizer for GPCP-SG (pr) (Pull request #3150) @FranziskaWinterstein
- Extension of NASA MERRA2 CMORizer (cl, cli, clivi, clw, clwvi) (Pull request #3167) @axel-lauer

# 63.6 Automatic testing

- Add a CircleCI-testing-specific recipe\_python\_for\_CI.yml to avoid calling geolocator/Nominatim over CI (Pull request #3159) @valeriupredoi
- Check if Python minor version changed after Julia install in development installation test (Pull request #3213) @valeriupredoi
- Fix tests using deprecated esmvalcore.\_config module that has been removed in ESMValCore v2.9 (Pull request #3204) @valeriupredoi

## 63.7 Installation

- Add support for Python=3.11 (Pull request #3173) @valeriupredoi
- Drop python=3.8 support (Pull request #3193) @valeriupredoi
- Repair generation of conda lock files (Pull request #3148) @valeriupredoi
- Modernize lock creation script and repair lock generation (Pull request #3174) @valeriupredoi
- Pin numpy !=1.24.3 due to severe masking bug (Pull request #3182) @valeriupredoi
- Update xesmf to versions >= 0.4.0 (Pull request #2728) @zklaus
- Update esmpy import for ESMF version 8.4.0 or larger (Pull request #3188) @valeriupredoi
- Relax the pin on iris to allow the use of older versions for performance reasons (Pull request #3270) @bouwe-andela
- Use ESMValCore v2.9.0 (Pull request #3274) @bouweandela

### 63.8 Improvements

- Update pre-commit hooks (Pull request #3189) @bouweandela
- Add support for using a dask distributed scheduler (Pull request #3151) @bouweandela

#### SIXTYFOUR

#### V2.8.0

#### 64.1 Highlights

- This release includes the diagnostics for reproducing figures 3.9, 3.19, 3.42 and 3.43 of the IPCC AR6 WG1 report. See *recipe documentation* about added recipes.
- A new set of recipes and diagnostics has been included to evaluate cloud climatologies from CMIP models as used in Lauer et al. (2023), J. Climate. See *recipe documentation* about added recipes.
- Addition of a set of recipes for extreme events, regional and impact evaluation as used in Weigel et al. (2021), J. Climate and in IPCC AR5. See *recipe documentation* about added recipes.

Highlights from ESMValCore v2.8.0 here:

- ESMValCore now supports wildcards in recipes and offers improved support for ancillary variables and dataset versioning.
- Support for CORDEX datasets in a rotated pole coordinate system has been added.
- Native ICON output is now made UGRID-compliant on-the-fly.
- The Python API has been extended with the addition of three modules: esmvalcore.config, esmvalcore.dataset, and esmvalcore.local
- The preprocessor multi\_model\_statistics() has been extended to support more use-cases.

This release includes:

#### 64.2 Backwards incompatible changes

Please read the descriptions of the linked pull requests for detailed upgrade instructions.

- Deprecated features scheduled for removal in v2.8.0 or earlier have now been removed (Pull request #2941) @schlunma. Removed esmvaltool.iris\_helpers.var\_name\_constraint (has been deprecated in v2.6.0; please use iris.NameConstraint with the keyword argument var\_name instead). Removed write\_netcdf and write\_plots from recipe\_filer.py.
- No files from the native6 project will be found if a non-existent version of a dataset is specified (#3041) @remikazeroni. The tool now searches for exact version of native6 datasets. Therefore, it is necessary to make sure that the version number in the directory tree matches with the version number in the recipe to find the files.
- The conversion of precipitation units from monitoring diagnostic is now done at the preprocessor stage (#3049) @schlunma. To use the unit conversion for precipitation in the new version of this diagnostic, add it as a preprocessor for the precipitation dataset to the recipe.

## 64.3 Bug fixes

- Fix for provenance records from seaice\_tsline.ncl (Pull request #2938) @axel-lauer
- Fix in *validation.py* for resolving datasets with identical names by using distinct aliases (Pull request #2955) @FranziskaWinterstein
- Bugfix: masking of non-significant differences in zonal.ncl (perfmetrics) (Pull request #2957) @axel-lauer
- Fix typo in perfmetrics/main.ncl to add tropopause (Pull request #2966) @FranziskaWinterstein
- Fix .png bug in wenzel16nat diagnostics (Pull request #2976) @axel-lauer
- *Recipe\_ocean\_Landschuetzer2016*: Fix typo in filename to run model vs OBS diagnostics (Pull request #2997) @TomasTorsvik
- Fix read\_cmor in NCL utilities (Pull request #3007) @axel-lauer
- Removed usages of deprecated features that cause diagnostic crashes (Pull request #3009) @schlunma
- Replace removed matplotlib.pyplot.savefig option additional\_artists (Pull request #3075) @schlunma
- Added missing comma to sommer17joss.bibtex (Pull request #3078) @schlunma
- Fix call of output\_type in *aux\_plotting.ncl* (Pull request #3083) @LisaBock
- Remove colorbar from *bbox\_extra\_artists* (Pull request #3087) @schlunma
- Fix MPI-ESM1-2-HR entries in recipe\_tebaldi21esd (Pull request #3093) @remi-kazeroni
- Fix bug in provenance writing of perfmetrics recipes v2.8.0 (Pull request #3098) @axel-lauer
- Fix recipe\_sea\_surface\_salinity for v2.8 (Pull request #3102) @sloosvel
- Fix variable short\_name and metadata for ESACCI-LST CMORizer (Pull request #3104) @remi-kazeroni
- Fix recipe\_carvalhais14: replace outline patch with splines (Pull request #3111) @valeriupredoi
- Replace deprecated function *cm.register\_cmap* with *mpl.colormaps.register* for *recipe\_arctic\_ocean* (Pull request #3112) @TomasTorsvik
- Fix recipe\_extract\_shape.yml (lacking caption for provenance) (Pull request #3126) @valeriupredoi

## 64.4 Community

• Update documentation on pre-installed versions on HPC clusters (Pull request #2934) @remi-kazeroni

## 64.5 Deprecations

• Remove radiation recipes that have been superseded by *recipe\_radiation\_budget* along with associated diagnostic scripts (#3115) @alistairsellar

#### 64.6 Documentation

- Backward compatibility policy (Pull request #2879) @alistairsellar
- Suppress installing and reinstalling dependencies with pip during readthedocs builds (Pull request #2913) @valeriupredoi
- Update installation instructions (Pull request #2939) @bouweandela
- Update documentation for recipe\_extreme\_index (Pull request #2951) @katjaweigel
- Update documentation and recipe\_check\_obs (ERA5) (Pull request #2952) @axel-lauer
- Updated ICON dataset entry in documentation (Pull request #2954) @schlunma
- Add Franziska Winterstein as collaborator in CITATION file (Pull request #3001) @valeriupredoi
- Update release schedule for v2.7.0 and v2.8.0 (Pull request #3010) @remi-kazeroni
- Add ESMValCore Bugfix release v2.7.1 to the release overview table (Pull request #3028) @valeriupredoi
- Detailed instructions for release procedure: running recipes and analyzing the output (Pull request #3032) @valeriupredoi
- Link backward compatibility policy to top level of ESMValCore changelog (Pull request #3052) @alistairsellar
- Update release instructions (Pull request #3066) @remi-kazeroni
- Updated docs and tests regarding new search\_esgf option (Pull request #3069) @schlunma
- Update script to draft release notes (Pull request #3070) @remi-kazeroni
- Synchronize documentation table of contents with ESMValCore (Pull request #3073) @bouweandela
- Update environment handling in release documentation (Pull request #3096) @remi-kazeroni
- Clarify use (or not) of Jasmin climatology files by soil moisture & permafrost recipes (Pull request #3103) @alistairsellar
- Add link to recipe portal in the gallery page (Pull request #3113) @remi-kazeroni
- Improve stratosphere documentation (Pull request #3114) @alistairsellar
- Added note to documentation that not all datasets used in *schlund20jgr* recipes are available on ESGF (Pull request #3121) @schlunma
- Draft changelog for v2.8.0 (Pull request #3124) @remi-kazeroni
- Documenting broken recipes after recipe testing for releases (Pull request #3129) @remi-kazeroni
- Increase ESMValTool version to 2.8.0 and update release dates (Pull request #3136) @remi-kazeroni

## 64.7 Diagnostics

- Cloud diagnostics for Lauer et al. (2023) (Pull request #2750) @axel-lauer
- Splitting of *flato13ipcc.yml* into separate recipes and adding recipes for regional Figures (Pull request #2156) @katjaweigel
- Adding IPCC AR6 Chapter 3 Figure 3.43 Pattern Correlation (Pull request #2772) @LisaBock
- Adding IPCC AR6 Chapter 3 Fig. 3.42 Perfmetrics (Pull request #2856) @LisaBock
- Comment missing datasets and remove deprecated argument in *recipe\_climate\_change\_hotspot* (Pull request #2920) @sloosvel

- Add plot type annual\_cycle to multi-dataset monitoring diagnostic (Pull request #2922) @schlunma
- Adding IPCC AR6 Chapter 3 Fig. 3.19 Speed-Up Of Zonal Mean Wind (Pull request #2984) @LisaBock
- Adding IPCC AR6 Chapter 3 Fig. 3.9 Attribution (Pull request #2986) @LisaBock
- Obs4mips CERES-EBAF: update version to latest available through esgf in *recipe\_validation.yml* (Pull request #3002) @valeriupredoi
- Improve flexibility of cloud diagnostics (Pull request #3016) @axel-lauer
- Let *recipe\_impact.yml* write a CSV file that can directly be used in C4I portal (Pull request #2258) @Peter9192
- Fix version numbers of native6 datasets in recipes (#3041) @remi-kazeroni
- Removed automatic conversion of precipitation units from monitoring diagnostic (#3049) @schlunma.
- Updated recipes for ESMValCore v2.8 (Pull request #3064) @schlunma
- Fix cos22esd for release of 2.8 (Pull request #3097) @sloosvel
- Diagnostic for *recipe\_autoassess\_stratosphere.yml*: remove unused feature incompatible with Matplotlib=3.7.1 (Pull request #3089) @valeriupredoi
- Fix numpy deprecation in hype diagnostic (Pull request #3101) @Peter9192
- Remove superseded radiation recipes (#3115) @alistairsellar
- Removed fx\_variables in recipe\_mpqb\_xch4 and recipe\_lauer22jclim\_fig8 (Pull request #3117) @axel-lauer
- Update Python example recipe (Pull request #3119) @bouweandela
- Updated figure settings to account for newer matplotlib version (Pull request #3133) @katjaweigel

## 64.8 Observational and re-analysis dataset support

- Earth System Data Cube (ESDC) cmorizer (Pull request #2799) @bsolino
- Added CMORizer for Landschützer2020 (spco2) (Pull request #2908) @schlunma
- Added CMORizer for MOBO-DIC\_MPIM (dissic) (Pull request #2909) @schlunma
- Added CMORizer for OceanSODA-ETHZ (areacello, co3os, dissicos, fgco2, phos, spco2, talkos) (Pull request #2915) @schlunma
- Extension of ERA-Interim CMORizer (cl, cli, clw, lwp, rlut, rlutcs, rsut, rsutcs) (Pull request #2923) @axel-lauer
- Add JRA-25 cmorizer (clt, hus, prw, rlut, rlutcs, rsut, rsutcs) (Pull request #2927) @LisaBock
- New CMORizers for datasets from the NCEP family (NCEP-DOE-R2, NCEP-NCAR-R1, NOAA-CIRES-20CR) (Pull request #2931) @hb326
- Updates to the recipes that use the NCEP reanalysis dataset (Pull request #2932) @hb326
- MERRA2 cmorizer convert vertical level coordinate units from hPa to Pa (Pull request #3003) @valeriupredoi
- MERRA2 cmorizer set UNLIMITED time coordinate (Pull request #3006) @valeriupredoi
- Added CMORizers for TCOM-CH4 (CH4) and TCOM-N2O (N2O) (Pull request #3014) @schlunma
- Update HadISST cmorizer to include recent years (Pull request #3027) @remi-kazeroni

#### 64.9 Automatic testing

- Add DKRZ/Levante batch scripts for release recipe running (Pull request #2883) @valeriupredoi
- Remove pytest-flake8 and call the use of flake8 straight (Pull request #2904) @valeriupredoi
- Unpin flake8 (Pull request #2937) @valeriupredoi
- Fix failing tests that use deprecated feature of sklearn (Pull request #2961) @schlunma
- Fix recipe loading tests for esmvalcore before and after version 2.8 (Pull request #3020) @valeriupredoi
- Update recipe load test for v2.8 (Pull request #3040) @bouweandela
- Test running recipes with the development version of ESMValCore (Pull request #3072) @bouweandela
- Fix test\_naming.py so it doesn't let through directories that need be ignored (Pull request #3082) @valeriupredoi
- Conda environment files for interim use of esmvalcore=2.8.0rc1 (Pull request #3090) @valeriupredoi
- Move *flake8* check to a step separate from installation on CircleCI (Pull request #3105) @bouweandela
- Recreate conda lock file to harpoon esmvalcore=2.8.0rc1 (Pull request #3108) @valeriupredoi
- Update batch script generation to run all recipes in one command (Pull request #3130) @remi-kazeroni

#### 64.10 Installation

- Merge release branch *release\_270stable* in main so we pick up unsquashed commits and set the correct version 2.7.0 for main (and up version in CITATION.cff) (Pull request #2896) @valeriupredoi
- Unpin NetCDF4 (Pull request #2929) @valeriupredoi
- Unpin cf-units (Pull request #2930) @bouweandela
- Set the version number on the development branches to one minor version more than the last release (Pull request #2964) @bouweandela
- Pin shapely<2.0.0 for linux64 (Pull request #2970) @valeriupredoi
- Unpin matplotlib (Pull request #3068) @valeriupredoi
- Add packaging as direct dependency to ESMValTool (Pull request #3099) @valeriupredoi
- Re-pin sphinx to latest (6.1.3) and add nbsphinx to the environment (Pull request #3118) @valeriupredoi
- Conda environment files for esmvalcore=2.8.0rc2 (Pull request #3120) @remi-kazeroni
- Remove rc (release candidates) conda channel and re-pin esmvalcore to new stable 2.8 (Pull request #3131) @valeriupredoi

### 64.11 Improvements

- Read config-user.yml using esmvalcore.config module (Pull request #2736) @bouweandela
- Make results of recipes schlund20jgr\_\*.yml deterministic (Pull request #2900) @schlunma
- Recipe\_gier2020bg.yml: add sorting to SA barplot (Pull request #2905) @bettina-gier
- Add the outline of a climatological tropopause to the zonalmean\_profile plots (Pull request #2947) @FranziskaWinterstein
- Update data finder imports (Pull request #2958) @bouweandela
- Add support for the upcoming ESMValCore v2.8 release to the recipe filler tool (Pull request #2995) @bouwe-andela
- Updated monitoring diagnostics with netCDF output and additional logging (Pull request #3029) @schlunma
- Use aliases in perfmetrics (Pull request #3058) @FranziskaWinterstein

#### SIXTYFIVE

#### V2.7.0

#### 65.1 Highlights

- This release has seen the inclusion of the code for figures 3.3, 3.4, 3.5, 3,13 and 3.15 of the IPCC AR6 WG1 report, see them in the new documentation
- We have also included new diagnostics and recipe necessary to produce the plots and tables for the journal article "Climate model projections from the Scenario Model Intercomparison Project (ScenarioMIP) of CMIP6" by Tebaldi et al. in ESD 2020-68 from 2021; also see the recipe entry
- We have also extended the support for MERRA2 observational dataset, by adding support for a large number of variables, including 3D variables, see the table of supported obs datasets

#### 65.2 Backwards incompatible changes

• Remove installation of R dependencies from the help message (Pull request #2761) @remi-kazeroni

## 65.3 Bug fixes

- Fix misplaced provenance records from IPCC AR5 Ch.12 diags (Pull request #2758) @axel-lauer
- Fix *esmvaltool.utils.testing.regression.compare* module to run with Python<3.10 too (Pull request #2778) @va-leriupredoi
- Fixed small bug that could lead to wrong pr units in monitor/multi\_datasets.py (Pull request #2788) @schlunma
- Pin xgboost>1.6.1 so we avert documentation failing to build with 1.6.1 (Pull request #2780) @valeriupredoi
- Pin *matplotlib-base*<3.6.0 to avoid conflict from *mapgenerator* that fails doc builds (Pull request #2830) @va-leriupredoi
- Fixed wrong latitudes in NDP CMORizer (Pull request #2832) @schlunma
- Fix indexer in Autoassess supermeans module use a tuple of (*slice(), idx, idx*) (Pull request #2838) @valeriupre-doi
- Replace xarray ufuncs with bogstandard numpy in weighting/climwip/calibrate\_sigmas.py (Pull request #2848) @valeriupredoi
- Fix units MERRA2 CMORizer (Pull request #2850) @axel-lauer
- Fix bug when using log-scale y-axis for ocean transects. (Pull request #2862) @TomasTorsvik

## 65.4 Community

• Add MO-paths to config file (Pull request #2784) mo-tgeddes

# 65.5 Deprecations

• Recipe *recipe\_esacci\_oc.yml* replace with new regrid scheme *nearest\_extrapolate* (Pull request #2841) @valeri-upredoi

## 65.6 Documentation

- Update release schedule for v2.7 (Pull request #2747) @bouweandela
- Add Met Office installation method (Pull request #2751) mo-tgeddes
- Add release dates for 2023 (Pull request #2769) @remi-kazeroni
- Made maintainer entry mandatory for published recipes (Pull request #2703) @schlunma
- Use command with current command line opts for *cffconvert* in documentation (Pull request #2791) @valeri-upredoi
- Update CMORizer documentation with command options (Pull request #2795) @remi-kazeroni
- Fixed broken link for monthly meetings (Pull request #2806) @remi-kazeroni
- Update MO obs4MIPs paths in the user configuration file (Pull request #2813) mo-tgeddes
- Fix Windows incompatible file names in documentation of recipe\_climate\_change\_hotspot.yml (Pull request #2823) @ledm
- Update documentation for the Landschuetzer 2016 recipe. (Pull request #2801) @TomasTorsvik
- Fixed anaconda badge in README (Pull request #2866) @valeriupredoi
- Update release strategy notes (Pull request #2734) @sloosvel
- Add documentation on how to handle CMORizers for multiple dataset versions (Pull request #2730) @remikazeroni
- Extending documentation: recipe maintainer + broken recipe policy (Pull request #2719) @axel-lauer

## 65.7 Diagnostics

- Recipe and diagnostics for : Tebaldi et al., ESD, 2021 (Pull request #2052) debe-kevin
- Figures for IPCC AR6 WG1 Chapter 3 (Atmosphere) (Pull request #2533) @LisaBock

### 65.8 Observational and re-analysis dataset support

- Update CERES-EBAF to Ed4.1 (Pull request #2752) @axel-lauer
- New CMORizer for CALIPSO-ICECLOUD (Pull request #2753) @axel-lauer
- New CMORizer for CLOUDSAT-L2 (Pull request #2754) @axel-lauer
- Update MERRA2 cmorizer with extra 2D and 3D variables (Pull request #2774) @valeriupredoi

## 65.9 Automatic testing

• Pin netcdf4 != 1.6.1 since that is spitting large numbers of SegFaults (Pull request #2796) @valeriupredoi

## 65.10 Installation

- Increase esmvalcore version to 2.7.0 in environment files (Pull request #2860) @valeriupredoi
- Add iris-esmf-regrid as a dependency (Pull request #2880) @zklaus

### 65.11 Improvements

- Fix tebaldi21esd (Pull request #2749) @axel-lauer
- Added option to show basic statistics in plots of monitor/multi\_datasets.py (Pull request #2790) @schlunma
- Remove retracted datasets from recipe\_climate\_change\_hotspot (Pull request #2854) @sloosvel

#### SIXTYSIX

#### V2.6.0

#### 66.1 Highlights

- A new monitoring diagnostic has been added to allow the comparison of model runs against reference datasets. For details, see *Monitoring diagnostic to show multiple datasets in one plot (incl. biases)*.
- A tool has been developed to compare the output of recipe runs against previous runs, in order to detect in an automated way breaking changes between releases. Find more information in *Comparing recipe runs*.
- The recipe Climate Change Hotspot allows to compute hotspots in any rectangular region.

Please also note the highlights from the corresponding ESMValCore release here. Thanks to that ESMValTool has gained the following features:

- A new set of CMOR fixes is now available in order to load native EMAC model output and CMORize it on the fly.
- The version number of ESMValCore is now automatically generated using setuptools\_scm, which extracts Python package versions from git metadata.

This release includes

#### 66.2 Bug fixes

- Fix dtype for Marrmot recipe results (Pull request #2646) @SarahAlidoost
- Adapt test\_fix\_coords to new version of cf-units (Pull request #2707) @zklaus
- Fix nested axes in recipe\_martin18\_grl and recipe\_li17natcc (Pull request #2712) @lukruh
- Update common\_climdex\_preprocessing\_for\_plots.R (Pull request #2727) @earnone

## 66.3 Community

• Collecting github user names for config-references (Pull request #2677) @lukruh

#### 66.4 Deprecations

• Deprecate the function *esmvaltool.diag\_scripts.shared.var\_name\_constraint*. This function is scheduled for removal in v2.8.0. Please use iris.NameConstraint with the keyword argument var\_name instead: this is an exact replacement. (Pull request #2655) @schlunma

#### 66.5 Documentation

- Documentation Improvements (Pull request #2580) @stacristo
- Fixed broken label in the documentation (Pull request #2616) @remi-kazeroni
- Add readthedocs configuration file (Pull request #2627) @bouweandela
- Update the command for building the documentation (Pull request #2622) @bouweandela
- Added DKRZ-Levante to config-user-example.yml (Pull request #2632) @remi-kazeroni
- Improved documentation on native dataset support (Pull request #2635) @schlunma
- Add documentation on building and uploading Docker images (Pull request #2662) @bouweandela
- Remove support for Mistral in config-user-example.yml (Pull request #2667) @remi-kazeroni
- Add note to clarify that CORDEX support is work in progress (Pull request #2682) @bouweandela
- Restore accidentally deleted text from input data docs (Pull request #2683) @bouweandela
- Add running settings note in recipe\_wenzel16nat.yml documentation (Pull request #2692) @sloosvel
- Add a note on transferring permissions to the release manager (Pull request #2688) @bouweandela
- Update documentation on ESMValTool module at DKRZ (Pull request #2696) @remi-kazeroni
- Add note on how to run recipe\_wenzel14jgr.yml (Pull request #2717) @sloosvel
- Added conda forge feedstock repo link in README (Pull request #2555) @valeriupredoi

#### 66.6 Diagnostics

- Compute bias instead of correlation in *compare\_salinity.py* (Pull request #2642) @sloosvel
- Update monitor diagnostics (Pull request #2608) @schlunma
- Add new Psyplot diagnostic (Pull request #2653) @schlunma
- Reduce memory usage of lisflood recipe (Pull request #2634) @sverhoeven
- Provenance in ocean diagnostics (Pull request #2651) @tomaslovato
- Extend monitor diagnostics with multi-dataset plots (Pull request #2657) @schlunma
- Recipe and diagnostics to plot climate change hotspots: Cos et al., ESD 2022 (Pull request #2614) @pepcos
- Update plots of consecutive dry days recipe (Pull request #2671) @bouweandela
- Fix the format of ids in Hype forcing files (Pull request #2679) @SarahAlidoost
- WFlow diagnostic script: remove manual rechunking (Pull request #2680) @Peter9192

### 66.7 Observational and re-analysis dataset support

- Extending the HadCRUT5 cmorizer (Pull request #2509) @LisaBock
- Cmorize Kadow2020 dataset (Pull request #2513) @LisaBock
- Cmorize NOAAGlobalTemp dataset (Pull request #2515) @LisaBock
- Add option to CMORize ts as tos in ESACCI data (Pull request #2731) @sloosvel

### 66.8 Automatic testing

- Add a tool for comparing recipe runs to previous runs (Pull request #2613) @bouweandela
- Ignore NCL interface files when comparing recipe runs (Pull request #2673) @bouweandela
- Add a short version of recipe deangelis15nat for testing (Pull request #2685) @katjaweigel
- Expanded recipe output comparison tool to better handle absolute paths in output (Pull request #2709) @schlunma
- Update development infrastructure (Pull request #2663) @bouweandela

## 66.9 Installation

• Removed package/meta.yaml and all references to it (Pull request #2612) @schlunma

#### 66.10 Improvements

- Improved handling of weights in MLR diagnostics (Pull request #2625) @schlunma
- Fixed order of variables in perfemetrics plot of Anav13jclim recipe (Pull request #2706) @schlunma
- Added input file sorting to many diagnostic to make output exactly reproducible (Pull request #2710) @schlunma
- Removed 'ancestors' attributes before saving netcdf files in emergent constraints diagnostics (Pull request #2713) @schlunma

#### SIXTYSEVEN

#### V2.5.0

#### 67.1 Highlights

- A new recipe to plot generic preprocessor output is now available. For details, see *Monitor*.
- The CMORization of observational and other datasets has been overhauled. For many datasets, an automatic download script is now available. For details, see *Observations* and *Writing a CMORizer script for an additional dataset*.

Please also note the highlights from the corresponding ESMValCore release here. Thanks to that ESMValTool has gained the following features:

- The new preprocessor extract\_location can extract arbitrary locations on the Earth.
- Time ranges can now be extracted using the ISO 8601 format.
- The new preprocessor ensemble\_statistics can calculate arbitrary statistics over all ensemble members of a simulation.

This release includes

#### 67.2 Backwards incompatible changes

- Streamline observations download (Pull request #1657) Javier Vegas-Regidor. This change removes the cmorize\_obs command which has previously been used to CMORize observations and other datasets. The new command esmvaltool data provides many new features apart from the CMORization (esmvaltool data format), for example, automatic downloading of observational datasets (esmvaltool data download). More details on this can be found *here* and *here*.
- Dropped Python 3.7 (Pull request #2585) @schlunma. ESMValTool v2.5.0 dropped support for Python 3.7. From now on Python >=3.8 is required to install ESMValTool. The main reason for this is that conda-forge dropped support for Python 3.7 for OSX and arm64 (more details are given here).

## 67.3 Bug fixes

- Remove the use of *esmvalgroup* channel from the conda install Github Action workflow (Pull request #2420) @valeriupredoi
- Ignore .pymon-journal file in test discovery (Pull request #2491) @zklaus
- Relocate pytest-monitor outputted database *.pymon* so *.pymon-journal* file should not be looked for by *pytest* (Pull request #2501) @valeriupredoi
- Re-establish Python 3.7 compatibility (Pull request #2506) @zklaus
- Update intersphinx mapping (Pull request #2531) @zklaus
- Fixed KeyError in recipe\_ocean\_bgc.yml (Pull request #2540) @schlunma
- Corrected ESACCI-SEA-SURFACE-SALINITY from OBS to OBS6 (Pull request #2542) @axel-lauer
- Fixed recipe\_kcs.yml (Pull request #2541) @schlunma
- Fix MDER diagnostic regression\_stepwise (Pull request #2545) @axel-lauer
- Fix for recipe\_wenzel16nat (Pull request #2547) @axel-lauer
- Fixed recipe\_carvalhais14nat and removed deprecated use of np.float (Pull request #2558) @schlunma
- Fix recipe\_wenzel14jgr (Pull request #2577) @remi-kazeroni
- Fixed various recipes by removing faulty or non-available datasets (Pull request #2563) @schlunma
- Remove missing CMIP5 data from 2 recipes (Pull request #2579) @remi-kazeroni
- Fix recipe\_seaice (Pull request #2578) @remi-kazeroni
- Fix recipe\_climwip\_brunner20esd (Pull request #2581) @remi-kazeroni

## **67.4 Deprecations**

- Remove *-use-feature=2020-resolver* command line option for obsolete pip 2020 solver (Pull request #2493) @valeriupredoi
- Renamed vertical regridding schemes in affected recipes (Pull request #2487) @schlunma

## 67.5 Documentation

- Update release manager for v2.5 (Pull request #2429) @axel-lauer
- Mention ENES Climate Analytics service (Pull request #2438) @bouweandela
- Add recipe overview page (Pull request #2439) @bouweandela
- Fix pointer to Tutorial lesson on preprocessor from 05 to 06 (Pull request #2473) @valeriupredoi
- Removed obsolete option synda-download from documentation (Pull request #2485) @schlunma
- Update CMUG XCH4 docu figure (Pull request #2502) @axel-lauer
- Add Python=3.10 to package info, update Circle CI auto install and documentation for Python=3.10 (Pull request #2503) @schlunma
- Unify user configuration file (Pull request #2507) @schlunma

- Synchronized config-user.yml with version from ESMValCore (Pull request #2516) @schlunma
- CITATION.cff fix and automatic validation of your citation metadata (Pull request #2517) @abelsiqueira
- Add backwards incompatible changes at the top of the release notes draft (Pull request #2431) @bouweandela
- Fixed intersphinx mapping of scipy (Pull request #2523) @schlunma
- Add authors to citation cff (Pull request #2525) @SarahAlidoost
- Update documentation on running a recipe (Pull request #2432) @bouweandela
- Fix recipe hydrology/recipe\_wflow.yml (Pull request #2549) @remi-kazeroni
- Update draft\_release\_notes.py for new release (Pull request #2553) @schlunma
- Added stand with Ukraine badge (Pull request #2565) @valeriupredoi
- Updated CREM docu (recipe\_williams09climdyn.yml) (Pull request #2567) @axel-lauer
- First draft for v2.5.0 changelog (Pull request #2554) @schlunma
- Replace nonfunctional Github Actions badge with cool one in README (Pull request #2582) @valeriupredoi
- Updated changelog (Pull request #2589) @schlunma
- Updated release strategy with current release and upcoming release (Pull request #2597) @schlunma
- Increased ESMValTool version to 2.5.0 (Pull request #2600) @schlunma

#### **67.6 Diagnostics**

- AutoAssess: Add new diagnostic for radiation budget (Pull request #2282) @Jon-Lillis
- CMUG Sea Surface Salinity dataset and diagnostic (Pull request #1832) Javier Vegas-Regidor
- Recipe with new diagnostics for ESA-CMUG H2O (Pull request #1834) @katjaweigel
- Cleaned Schlund et al. (2020) recipe and fixed small bugs in corresponding diagnostic (Pull request #2484) @schlunma
- Add ESA CCI LST cmorizer and diagnostic (Pull request #1897) @morobking
- XCH4 ESA CMUG diagnostics (subset of the MPQB diagnostics) (Pull request #1960) @hb326
- Add support for ESACCI Ocean Color (Chlorophyll) observations (Pull request #2055) ulrikaw-cloud
- Updated recipe\_zmnam.yml with hemisphere selection (Pull request #2230) @fserva
- Add recipe and diagnostic scripts to compute figures of D9.4 of ISENES3 (Pull request #2441) @sloosvel
- Save resampled climates from KCS diagnostic local\_resampling.py (Pull request #2221) @Emmadd
- Use years from KCS recipe (Pull request #2223) @Emmadd
- Recipe to plot generic output from the preprocessor (Pull request #2184) Javier Vegas-Regidor
- Fixed provenance tracking for emergent constraint diagnostics (Pull request #2573) @schlunma

## 67.7 Observational and re-analysis dataset support

- Ensure dummy data for cmorize\_obs\_woa test are written to the correct directory (Pull request #2451) @ehogan
- Add ESA CCI LST cmorizer and diagnostic (see previous section *Diagnostics*)

# 67.8 Automatic testing

- Run a nightly Github Actions workflow to monitor tests memory per test (configurable for other metrics too) and lists the slowest 100 tests (Pull request #2449) @valeriupredoi
- Fix individual pytest runs broken due to missing explicit imports from *iris* and adding a couple missing package markers (Pull request #2455) @valeriupredoi
- Add Python=3.10 to Github Actions and switch to Python=3.10 for the Github Action that builds the PyPi package (Pull request #2488) @valeriupredoi
- Switch all github actions from miniconda to mambaforge (Pull request #2498) @zklaus
- Pin *flake8*<4 to have actual FLAKE8 error printed if tests fail and not garbage (Pull request #2492) @valeriupre-doi
- Implementing conda lock (Pull request #2193) @valeriupredoi
- [Docker] Update Docker container builds with correct installations of Julia (Pull request #2530) @valeriupredoi
- Update Linux condalock file (various pull requests) github-actions[bot]

## 67.9 Installation

- Comment out release candidate channel in environment.yml (Pull request #2417) @zklaus
- Comment out rc channel in osx environment file (Pull request #2421) @valeriupredoi
- Add *python-cdo* as conda-forge dependency in environment files to ensure *cdo* gets used from conda-forge and not pip (Pull request #2469) @valeriupredoi
- Install rasterio from conda-forge and avoid issues from python=3.10 (Pull request #2479) @valeriupredoi
- Updated dependencies with new ESMValCore version (Pull request #2599) @schlunma

## 67.10 Improvements

- Remove use of OBS and use CMIP instead in examples/recipe\_ncl.yml (Pull request #2494) @valeriupredoi
- Expanded *recipe\_preprocessor\_test.yml* to account for new *multi\_model\_statistics* features (Pull request #2519) @schlunma
- Updated piControl periods for recipes that use KACE-1-0-G (Pull request #2537) @schlunma
- Reduced time range in recipe\_globwat.yml (Pull request #2548) @schlunma
- Removed models with missing data from recipe\_williams09climdyn.yml (Pull request #2566) @axel-lauer
- Restored original versions of *recipe\_schlund20esd.yml* and *recipe\_meehl20sciadv.yml* (Pull request #2583) @schlunma

#### SIXTYEIGHT

#### V2.4.0

#### **68.1 Highlights**

• ESMValTool is moving from Conda to Mamba as the preferred installation method. This will speed up the installation and comes with some improvements behind the scenes. Read more about it at *Move to Mamba* and in *the installation guide*.

Please also note the highlights from the corresponding ESMValCore release here. Thanks to that ESMValTool has gained the following features:

- Download any missing data that is available on the ESGF automatically.
- Resume previous runs, reusing expensive pre-processing results.

This release includes

#### 68.2 Bug fixes

- Fixed recipe\_meehl20sciadv.yml for ESMValCore 2.3 (Pull request #2253) @schlunma
- Fix provenance of NCL figures created using the log\_provenance function (Pull request #2279) @bouweandela
- Fix bug in ClimWIP brunner19 recipe when plotting (Pull request #2226) @lukasbrunner
- Pin docutils <0.17 to fix sphinx build with rtd theme (Pull request #2312) @zklaus
- Fix example recipes (Pull request #2338) @valeriupredoi
- Do not add bounds to plev (plev19) in era interim cmorizer (Pull request #2328) @valeriupredoi
- Fix problem with pip 21.3 that prevents installation from source (Pull request #2344) @zklaus
- Add title to recipe embedded in test\_diagnostic\_run.py (Pull request #2353) @zklaus
- Fix capitalization of obs4MIPs (Pull request #2368) @bouweandela
- Specify that areacella is needed for area statistics in the Python example recipe (Pull request #2371) @bouweandela
- Enabling variable obs550lt1aer in recipes (Pull request #2388) @remi-kazeroni
- Update a diagnostic to new Iris version (Pull request #2390) @katjaweigel
- Fixed bug in provenance tracking of ecs\_scatter.ncl (Pull request #2391) @schlunma
- Fix provenance issue in pv\_capacity\_factor.R (Pull request #2392) @katjaweigel
- Remove obsolete write\_plots option from R diagnostics (Pull request #2395) @zklaus

- Fix arctic ocean diagnostic (Pull request #2397) @zklaus
- Fix sea ice drift recipe and script (Pull request #2404) @sloosvel
- Adapt diagnostic script to new version of iris (Pull request #2403) @zklaus
- Fix ocean multimap (Pull request #2406) @zklaus
- Fix diagnostic that uses *xarray*: *dtype* correctly set and harmonize *xarray* and *matplotlib* (Pull request #2409) @zklaus
- Deactivate provenance logging for plots in thermodyn toolbox (Pull request #2414) @zklaus

## 68.3 Deprecations

- Removed write\_plots and write\_netcdf from some NCL diagnostics (Pull request #2293) @ schlunma
- Fixed provenance logging of all python diagnostics by removing 'plot\_file' entry (Pull request #2296) @schlunma
- Do not deprecate classes Variable, Variables and Datasets on a specific version (Pull request #2286) @schlunma
- Remove obsolete write\_netcdf option from ncl diagnostic scripts (Pull request #2387) @zklaus
- Remove write plots from ocean diagnostics (Pull request #2393) @valeriupredoi
- More removals of instances of *write\_plots* from Python diagnostics (appears to be the final removal from Py diags) (Pull request #2394) @valeriupredoi

#### 68.4 Documentation

- List Manuel Schlund as release manager for v2.5 (Pull request #2268) @bouweandela
- GlobWat fix download links and gdal command (Pull request #2334) @babdollahi
- Add titles to recipes authored by predoi\_valeriu (Pull request #2333) @valeriupredoi
- Added titles to recipes maintained by lauer\_axel (Pull request #2332) @axel-lauer
- Update the documentation of the GRACE CMORizer (Pull request #2349) @remi-kazeroni
- Add titles in BSC recipes (Pull request #2351) @sloosvel
- Update esmvalcore dependency to 2.4.0rc1 (Pull request #2348) @zklaus
- Add titles to recipes maintained by Peter Kalverla (Pull request #2356) @Peter9192
- Adding titles to the recipes with maintainer hb326 (Pull request #2358) @hb326
- Add title for zmnam as for #2354 (Pull request #2363) @fserva
- Added recipe titles the the ocean recipes. (Pull request #2364) @ledm
- Update recipe\_thermodyn\_diagtool.yml add title (Pull request #2365) @ValerioLembo
- Fix provenance of figures of several R diagnostics (Pull request #2300) @bouweandela
- Adding titles to Mattia's recipes (Pull request #2367) @remi-kazeroni
- Adding titles to wenzel recipes (Pull request #2366) @hb326
- Fix formatting of some recipe titles merged from PR 2364 (Pull request #2372) @zklaus
- Adding titles to Bjoern's recipes (Pull request #2369) @remi-kazeroni

- Add titles to ocean recipes (maintainer Lovato) (Pull request #2375) @tomaslovato
- Add titles for three c3s-magic recipes (Pull request #2378) @zklaus
- Add title for recipe maintained by Ruth Lorenz (Pull request #2379) @zklaus
- Fix toymodel recipe (Pull request #2381) Javier Vegas-Regidor
- Added titles for recipes of maintainer schlund\_manuel (Pull request #2377) @schlunma
- Write\_plots and titles for deangelis15nat, li17natcc, martin18grl, pv\_capacity\_factor (Pull request #2382) @kat-jaweigel
- Add titles for some recipes (Pull request #2383) @zklaus
- Adding titles for recipes by von Hardenberg and Arnone (Pull request #2384) @zklaus
- Last two missing titles (Pull request #2386) @valeriupredoi
- Update documentation on downloading data (Pull request #2370) @bouweandela
- Fix installation instructions for Julia (Pull request #2335) @zklaus
- Fix provenance of Julia example diagnostic (Pull request #2289) @bouweandela
- Added notes on use of mamba in the installation documentation chapter (Pull request #2236) @valeriupredoi
- Update version number for 2.4.0 release (Pull request #2410) @zklaus
- Update release schedule for 2.4.0 (Pull request #2412) @zklaus
- Update changelog for 2.4.0 release (Pull request #2411) @zklaus

## 68.5 Diagnostics

- Add all available CMIP5 and CMIP6 models to recipe\_impact.yml (Pull request #2251) @bouweandela
- Add Fig. 6, 7 and 9 of Bock20jgr (Pull request #2252) @LisaBock
- Generalize *recipe\_validation*\* diagnostic to work with identical control and experiment dataset names (Pull request #2284) @valeriupredoi
- Add missing preprocessor to recipe\_gier2020bg and adapt to available data (Pull request #2399) @bettina-gier
- Removed custom version of AtmosphereSigmaFactory in diagnostics (Pull request #2405) @schlunma

#### 68.6 Observational and re-analysis dataset support

- Replace recipe\_era5.yml with recipe\_daily\_era5.yml (Pull request #2182) @SarahAlidoost
- Update WOA cmorizer for WOA18 and WOA13v2 (Pull request #1812) @LisaBock
- GLODAP v2.2016 ocean data cmorizer (Pull request #2185) @tomaslovato
- Updated GCP CMORizer (Pull request #2295) @schlunma

### 68.7 Automatic testing

- Add a cylc suite to run all recipes (Pull request #2219) @bouweandela
- Retire test with Python 3.6 from full development Github Actions test (Pull request #2229) @valeriupredoi
- Remove Python 3.6 tests from GitHub Actions (Pull request #2264) @valeriupredoi
- Unpin upper bound for iris (previously was at <3.0.4) (Pull request #2266) @valeriupredoi
- Pin latest esmvalcore to allow use of the bugfix release 2.3.1 always (Pull request #2269) @valeriupredoi
- Add apt update so Julia gets found and installed by Docker (Pull request #2290) @valeriupredoi
- Use mamba for environment update and creation in the Docker container build on DockerHub (Pull request #2297) @valeriupredoi
- Docker container experimental run a full env solve with mamba instead of a conda update (Pull request #2306) @valeriupredoi
- Full use of mamba in Github Actions source install test and use generic Python 3.7 (removing the very specific 3.7.10) (Pull request #2287) @valeriupredoi
- Replace use of conda with mamba for conda\_install test on Circle CI (Pull request #2237) @valeriupredoi
- Update circleci configuration (Pull request #2357) @zklaus

## 68.8 Installation

• Remove mpich from conda dependencies list (Pull request #2343) @valeriupredoi

#### 68.9 Improvements

- Add script for extracting a list of input files from the provenance (Pull request #2278) @bouweandela
- Update github actions (Pull request #2360) @zklaus
- Removed 'write\_plots' from all NCL diagnostics (Pull request #2331) @axel-lauer
- Update and modernize config-user-example.yml (Pull request #2374) @valeriupredoi

#### SIXTYNINE

#### V2.3.0

This release includes

#### 69.1 Bug fixes

- Indent block to pick up and raise exception if cmorizer data not found (TierX dir is not there) (Pull request #1877) @valeriupredoi
- Skip recipe filler tests until we have a new release since GA tests are failing (Pull request #2089) @valeriupredoi
- Fixed broken link to contributions in README (Pull request #2102) @schlunma
- Fix recipe filler for the case the variable doesn't contain short\_name (Pull request #2104) @valeriupredoi
- Add fix for iris longitude bug to ClimWIP (Pull request #2107) @lukasbrunner
- Update for outdated link to reference Déandreis et al. (2014). (Pull request #2076) @katjaweigel
- Fixed recipes for ESMValCore 2.3.0 (Pull request #2203) @schlunma
- Fix the WFDE5 cmorizer (Pull request #2211) @remi-kazeroni
- Fix broken CMORizer log message if no Tier directory exists (Pull request #2207) @jmrgonza
- Fix bug in ClimWIP basic test recipe when plotting (Pull request #2225) @lukasbrunner
- Fix bug in ClimWIP advanced test recipe when plotting (Pull request #2227) @lukasbrunner
- Adjust time range for the WDFE5 dataset in the recipe\_check\_obs.yml (Pull request #2232) @remi-kazeroni
- Fix plot and provenance of recipe\_consecdrydays (Pull request #2244) @bouweandela

#### 69.2 Documentation

- Improving the README.md file with a more appealing look and bit more info (Pull request #2065) @valeri-upredoi
- Update plot title martin18grl (Pull request #2080) @katjaweigel
- Update contribution guidelines (Pull request #2031) @bouweandela
- Update links in pull request template to point to latest documentation (Pull request #2083) @bouweandela
- Update release schedule (Pull request #2081) @bouweandela
- Updates to contribution guidelines (Pull request #2092) @bouweandela
- Update documentation for ERA5 with new variables (Pull request #2111) @lukasbrunner

- Add OSX installation instructions to docs (Pull request #2115) @bvreede
- Instructions to use pre-installed versions on HPC clusters (Pull request #2197) @remi-kazeroni
- Add functional Autoassess diagnostics: land surface metrics: permafrost, soil moisture, surface radiation (Pull request #2170) @valeriupredoi
- Add citation info in *recipe\_eady\_growth\_rate.yml* (Pull request #2188) @sloosvel
- Update version number to 2.3.0 (Pull request #2213) @zklaus
- Update release schedule for 2.3.0 (Pull request #2247) @zklaus
- Changelog update to v2.3.0 (Pull request #2214) @zklaus

### **69.3 Diagnostics**

- Added figures 8 and 10 to recipe\_bock20jgr.yml (Pull request #2074) @schlunma
- Add hydrological forcing comparison recipe (Pull request #2013) @stefsmeets
- Added recipe for Meehl et al., Sci. Adv. (2020) (Pull request #2094) @schlunma
- Add GlobWat recipe and diagnostic (Pull request #1808) @babdollahi
- Add ClimWIP recipe to reproduce Brunner et al. 2019 (Pull request #2109) @lukasbrunner
- Update Climwip recipe to reproduce brunner2020esd (Pull request #1859) @ruthlorenz
- Update recipe\_thermodyn\_diagtool.yml: code improvements and more user options (Pull request #1391) @ValerioLembo
- Remove model AWI-CM-1-1-MR from recipe\_impact.yml (Pull request #2238) @bouweandela
- PV capacity factor for ESMValTool GMD paper (Pull request #2153) @katjaweigel

#### 69.4 Observational and re-analysis dataset support

- Cmorize wfde5 (Pull request #1991) @mwjury
- Make cmorizer utils funcs public in utilities.py and add some numpy style docstrings (Pull request #2206) @valeriupredoi
- CMORizer for CLARA-AVHRR cloud data (Pull request #2101) @axel-lauer
- Update of ESACCI-CLOUD CMORizer (Pull request #2144) @axel-lauer

#### 69.5 Automatic testing

- Force latest Python in empty environment in conda install CI test (Pull request #2069) @valeriupredoi
- Removed imports from private sklearn modules and improved test coverage of custom\_sklearn.py (Pull request #2078) @schlunma
- Move private \_(global)\_stock\_cube from esmvacore.preprocessor.\_regrid to cmorizer (Pull request #2087) @valeriupredoi
- Try mamba install esmvaltool (Pull request #2125) @valeriupredoi

- Reinstate OSX Github Action tests (Pull request #2110) @valeriupredoi
- Pin mpich to avoid default install of 3.4.1 and 3.4.2 with external\_0 builds (Pull request #2220) @valeriupredoi
- Include test sources in distribution (Pull request #2234) @zklaus
- Pin iris<3.0.4 to ensure we still (sort of) support Python 3.6 (Pull request #2246) @valeriupredoi

# 69.6 Installation

- Fix conda build by skipping documentation test (Pull request #2058) Javier Vegas-Regidor
- Update pin on esmvalcore pick up esmvalcore=2.3.0 (Pull request #2200) @valeriupredoi
- Pin Python to 3.9 for development installation (Pull request #2208) @bouweandela

## **69.7 Improvements**

- Add EUCP and IS-ENES3 projects to config-references (Pull request #2066) @Peter9192
- Fix flake8 tests on CircleCI (Pull request #2070) @bouweandela
- Added recipe filler. (Pull request #1707) @ledm
- Update use of fx vars to new syntax (Pull request #2145) @sloosvel
- Add recipe for climate impact research (Pull request #2072) @Peter9192
- Update references "master" to "main" (Pull request #2172) @axel-lauer
- Force git to ignore VSCode workspace files (Pull request #2186) Javier Vegas-Regidor
- Update to new ESMValTool logo (Pull request #2168) @axel-lauer
- Python cmorizers for CDR1 and CDR2 ESACCI H2O (TCWV=prw) data. (Pull request #2152) @katjaweigel
- Remove obsolete conda package (closes #2100) (Pull request #2103) @zklaus

#### SEVENTY

#### V2.2.0

#### 70.1 Highlights

ESMValTool is now using the recently released Iris 3. We acknowledge that this change may impact your work, as Iris 3 introduces several changes that are not backward-compatible, but we think that moving forward is the best decision for the tool in the long term.

This release includes

### 70.2 Bug fixes

- Bugfix: time weights in time\_operations (Pull request #1956) @axel-lauer
- Fix issues with bibtex references (Pull request #1955) @stefsmeets
- Fix ImportError for configure\_logging (Pull request #1976) @stefsmeets
- Add required functional parameters for extract time in recipe\_er5.yml (Pull request #1978) @valeriupredoi
- Revert "Fix ImportError for configure\_logging" (Pull request #1992) @bouweandela
- Fix import of esmvalcore \_logging module in cmorize\_obs.py (Pull request #2020) @valeriupredoi
- Fix logging import in cmorize\_obs again since last merge was nulled by pre-commit hooks (Pull request #2022) @valeriupredoi
- Refactor the functions in derive\_evspsblpot due to new iris (Pull request #2023) @SarahAlidoost
- Avoid importing private ESMValCore functions in CMORizer (Pull request #2027) @bouweandela
- Fix extract\_seasons in validation recipe (Pull request #2054) Javier Vegas-Regidor

#### 70.3 Deprecations

- Deprecate classes Variable, Variables and Datasets (Pull request #1944) @schlunma
- Python 3.9: remove pynio as dependency and replace with rasterio and pin Matplotlib>3.3.1 and pin cartopy>=0.18 (Pull request #1997) @valeriupredoi
- Removed write\_plots and write\_netcdf in some python diagnostics (Pull request #2036) @schlunma

### 70.4 Documentation

- Update instructions on making a release (Pull request #1867) @bouweandela
- Update review.rst (Pull request #1917) @axel-lauer
- Add guidance on how to review a pull request (Pull request #1872) @bouweandela
- Adding tutorial links to documentation (Pull request #1927) @hb326
- Added bibtex file for schlund20jgr (Pull request #1928) @schlunma
- Documentation contact added the actual email for the mailing list (Pull request #1938) @valeriupredoi
- Make CircleCI badge specific to main branch (Pull request #1831) @bouweandela
- Documentation on how to move code from a private repository to a public repository (Pull request #1920) @hb326
- Refine pull request review guidelines (Pull request #1924) @stefsmeets
- Update release schedule (Pull request #1948) @zklaus
- Improve contact info and move to more prominent location (Pull request #1950) @bouweandela
- Add some maintainers to some recipes that are missing them (Pull request #1970) @valeriupredoi
- Update core team info (Pull request #1973) @axel-lauer
- Combine installation from source instructions and add common issues (Pull request #1971) @bouweandela
- Update iris documentation URL for sphinx (Pull request #2003) @bouweandela
- Fix iris documentation link(s) with new iris3 location on readthedocs (Pull request #2012) @valeriupredoi
- Document how to run tests for installation verification (Pull request #1847) @valeriupredoi
- List Remi Kazeroni as a code owner and sole merger of CMORizers (Pull request #2017) @bouweandela
- Install documentation: mention that we build conda package with python>=3.7 (Pull request #2030) @valeri-upredoi
- Recipe and documentation update for ERA5-Land. (Pull request #1906) @katjaweigel
- Update changelog and changelog tool for v2.2.0 (Pull request #2043) Javier Vegas-Regidor
- Final update to the changelog for v2.2.0 (Pull request #2056) Javier Vegas-Regidor

## 70.5 Diagnostics

- Add mapplot diagnostic to ClimWIP (Pull request #1864) @lukasbrunner
- Add the option to weight variable groups in ClimWIP (Pull request #1856) @lukasbrunner
- Implementation of ensemble member recognition to the ClimWIP diagnostic (Pull request #1852) @lukasbrunner
- Restructure ClimWIP (Pull request #1919) @lukasbrunner
- Diagnostic for recipe\_eyring13jgr.yml Fig. 12 (Pull request #1922) @LisaBock
- Added changes in shared functions necessary for schlund20esd (Pull request #1967) @schlunma
- Adding recipe and diagnostics for Gier et al 2020 (Pull request #1914) @bettina-gier
- Added recipe, diagnostics and documentation for Schlund et al., ESD (2020) (Pull request #2015) @schlunma

- Add PRIMAVERA Eady Growth Rate diagnostic (Pull request #1285) @sloosvel
- Implement shape parameter calibration for ClimWIP (Pull request #1905) @lukasbrunner

#### 70.6 Observational and re-analysis dataset support

- Extended ESRL cmorizer (Pull request #1937) @bettina-gier
- Cmorizer for GRACE data (Pull request #1694) @bascrezee
- Cmorizer for latest ESACCI-SST data (Pull request #1895) @valeriupredoi
- Fix longitude in ESRL cmorizer (Pull request #1988) @bettina-gier
- Selectively turn off fixing bounds for coordinates during cmorization with utilities.py (Pull request #2014) @valeriupredoi
- Cmorize hadcrut5 (Pull request #1977) @mwjury
- Cmorize gpcc masking (Pull request #1995) @mwjury
- Cmorize\_utils\_save\_1mon\_Amon (Pull request #1990) @mwjury
- Cmorize gpcc fix (Pull request #1982) @mwjury
- Fix flake8 raised by develop test in cmorize\_obs\_gpcc.py (Pull request #2038) @valeriupredoi

#### 70.7 Automatic testing

- Switched miniconda conda setup hooks for Github Actions workflows (Pull request #1913) @valeriupredoi
- Fix style issue (Pull request #1929) @bouweandela
- Fix mlr test with solution that works for CentOS too (Pull request #1936) @valeriupredoi
- Temporary deactivation Github Actions on OSX (Pull request #1939) @valeriupredoi
- Fix conda installation test on CircleCI (Pull request #1952) @bouweandela
- Github Actions: change time for cron job that installs from conda (Pull request #1969) @valeriupredoi
- CI upload relevant artifacts for test job (Pull request #1999) @valeriupredoi
- Github Actions test that runs with the latest ESMValCore main (Pull request #1989) @valeriupredoi
- Introduce python 39 in Github Actions tests (Pull request #2029) @valeriupredoi
- Remove test for conda package installation on Python 3.6 (Pull request #2033) @valeriupredoi
- Update codacy coverage reporter to fix coverage (Pull request #2039) @bouweandela

## 70.8 Installation

- Simplify installation of R development dependencies (Pull request #1930) @bouweandela
- Fix docker build (Pull request #1934) @bouweandela
- Use new conda environment for installing ESMValTool in Docker containers (Pull request #1993) @bouweandela
- Fix conda build (Pull request #2026) @bouweandela

## 70.9 Improvements

- Allow multiple references for a cmorizer script (Pull request #1953) @SarahAlidoost
- Add GRACE to the recipe check\_obs (Pull request #1963) @remi-kazeroni
- Align ESMValTool to ESMValCore=2.2.0 (adopt iris3, fix environment for new Core release) (Pull request #1874) @stefsmeets
- Make it possible to use write\_plots and write\_netcdf from recipe instead of config-user.yml (Pull request #2018) @bouweandela
- Revise lisflood and hype recipes (Pull request #2035) @SarahAlidoost
- Set version to 2.2.0 (Pull request #2042) Javier Vegas-Regidor

## SEVENTYONE

### V2.1.1

This release includes

# 71.1 Improvements

- Fix the conda build on CircleCI (Pull request #1883) @bouweandela
- Pin matplotlib to <3.3 and add compilers (Pull request #1898) @bouweandela
- Pin esmvaltool subpackages to the same version and build as the esmvaltool conda package (Pull request #1899) @bouweandela

### 71.2 Documentation

• Release notes v2.1.1 (Pull request #1932) @valeriupredoi

## SEVENTYTWO

#### V2.1.0

This release includes

## 72.1 Diagnostics

- Add extra steps to diagnostic to make output of hydrology/recipe\_lisflood.yml usable by the LISFLOOD model (Pull request #1737) @JaroCamphuijsen
- Recipe to reproduce the 2014 KNMI Climate Scenarios (kcs). (Pull request #1667) @Peter9192
- Implement the climwip weighting scheme in a recipe and diagnostic (Pull request #1648) @JaroCamphuijsen
- Remove unreviewed autoassess recipes (Pull request #1840) @valeriupredoi
- Changes in shared scripts for Schlund et al., JGR: Biogeosciences, 2020 (Pull request #1845) @schlunma
- Updated derivation test recipe (Pull request #1790) @schlunma
- Support for multiple model occurrence in perf main (Pull request #1649) @bettina-gier
- Add recipe and diagnostics for Schlund et al., JGR: Biogeosciences, 2020 (Pull request #1860) @schlunma
- Adjust recipe\_extract\_shape.yml to recent changes in the example diagnostic.py (Pull request #1880) @bouwe-andela

## 72.2 Documentation

- Add pip installation instructions (Pull request #1783) @bouweandela
- Add installation instruction for R and Julia dependencies tot pip install (Pull request #1787) @bouweandela
- Avoid autodocsumm 0.2.0 and update documentation build dependencies (Pull request #1794) @bouweandela
- Add more information on working on cluster attached to ESGF node (Pull request #1821) @bouweandela
- Add release strategy to community documentation (Pull request #1809) @zklaus
- Update esmvaltool run command everywhere in documentation (Pull request #1820) @bouweandela
- Add more info on documenting a recipe (Pull request #1795) @bouweandela
- Improve the Python example diagnostic and documentation (Pull request #1827) @bouweandela
- Improve description of how to use draft\_release\_notes.py (Pull request #1848) @bouweandela
- Update changelog for release 2.1 (Pull request #1886) @valeriupredoi

### 72.3 Improvements

- Fix R installation in WSL (Pull request #1789) Javier Vegas-Regidor
- Add pre-commit for linting/formatting (Pull request #1796) @stefsmeets
- Speed up tests on CircleCI and use pytest to run them (Pull request #1804) @bouweandela
- Move pre-commit excludes to top-level and correct order of lintr and styler (Pull request #1805) @stefsmeets
- Remove isort setup to fix formatting conflict with yapf (Pull request #1815) @stefsmeets
- GitHub Actions (Pull request #1806) @valeriupredoi
- Fix yapf-isort import formatting conflict (Pull request #1822) @stefsmeets
- Replace vmprof with vprof as the default profiler (Pull request #1829) @bouweandela
- Update ESMValCore v2.1.0 requirement (Pull request #1839) Javier Vegas-Regidor
- Pin iris to version 2 (Pull request #1881) @bouweandela
- Pin eccodes to not use eccodes=2.19.0 for cdo to work fine (Pull request #1869) @valeriupredoi
- Increase version to 2.1.0 and add release notes (Pull request #1868) @valeriupredoi
- Github Actions Build Packages and Deploy tests (conda and PyPi) (Pull request #1858) @valeriupredoi

# 72.4 Observational and re-analysis dataset support

• Added CMORizer for Scripps-CO2-KUM (Pull request #1857) @schlunma

## CHAPTER SEVENTYTHREE

#### V2.0.0

This release includes

#### 73.1 Bug fixes

- Fix pep8-naming errors and fix zmnam diagnostic (Pull request #1702) @bouweandela
- Fix keyword argument in cmorize\_obs (Pull request #1721) @mattiarighi
- Fixed JMA-TRANSCOM CMORizer (Pull request #1735) @schlunma
- Fix bug in extract\_doi\_value (Pull request #1734) @bascrezee
- Fix small errors in the arctic\_ocean diagnostic (Pull request #1722) @koldunovn
- Flatten ancestor lists for diag\_spei.R and diag\_spi.R. (Pull request #1745) @katjaweigel
- Fix for recipe\_ocean\_ice\_extent.yml (Pull request #1744) @mattiarighi
- Fix recipe\_combined\_indices.yml provenance (Pull request #1746) Javier Vegas-Regidor
- Fix provenance in recipe\_multimodel\_products (Pull request #1747) Javier Vegas-Regidor
- Exclude FGOALS-g2 due to ESMValCore issue #728 (Pull request #1749) @mattiarighi
- Fix recipe\_modes\_of\_variability (Pull request #1753) Javier Vegas-Regidor
- Flatten lists for ancestors for hyint to prevent nested lists. (Pull request #1752) @katjaweigel
- Fix bug in cmorize\_obs\_eppley\_vgpm\_modis.py (#1729) (Pull request #1759) @tomaslovato
- Correct mip for clltkisccp in example derive preprocessor recipe (Pull request #1768) @bouweandela
- Update date conversion in recipe\_hype.yml (Pull request #1769) @bouweandela
- Fix recipe\_correlation.yml (Pull request #1767) @bouweandela
- Add attribute positive: down to plev coordinate in ERA-Interim CMORizer (Pull request #1771) @bouweandela
- Fix sispeed in recipe\_preprocessor\_derive\_test (Pull request #1772) Javier Vegas-Regidor
- Fix extreme events and extreme index ancestors (Pull request #1774) @katjaweigel
- Correct date in output filenames of ERA5 CMORizer recipe (Pull request #1773) @bouweandela
- Exclude WOA from multi-model stats in recipe\_ocean\_bgc (Pull request #1778) @mattiarighi

## 73.2 Diagnostics

- Enhancement of the hyint recipe to include etccdi indices (Pull request #1133) @earnone
- Add lazy regridding for wflow diagnostic (Pull request #1630) @bouweandela
- Miles default domains to include lat=0 (Pull request #1626) @jhardenberg
- Miles: selection of reference dataset based on experiment (Pull request #1632) @jhardenberg
- New recipe/diagnostic: recipe\_li17natcc.yml for Axels GMD Paper (Pull request #1567) @katjaweigel
- New recipe/diagnostics: recipe\_deangelis\_for\_gmdpart4.yml for Axels GMD Paper (Pull request #1576) @katjaweigel
- EWaterCycle: Add recipe to prepare input for LISFLOOD (Pull request #1298) @sverhoeven
- Use area weighted regridding in wflow diagnostic (Pull request #1643) @bouweandela
- Workaround for permetrics recipe until Iris3 (Pull request #1674) @mattiarighi
- C3S\_511\_MPQB\_bas-features (Pull request #1465) @bascrezee
- Additional Land perfmetrics (Pull request #1641) @bettina-gier
- Necessary diagnostic from eyring06jgr for the release of version2 (Pull request #1686) @hb326
- Drought characteristics based on Martin2018 and SPI for gmd paper (Pull request #1689) @katjaweigel
- Additional features and bugfixes for recipe anav13clim (Pull request #1723) @bettina-gier
- Gmd laueretal2020 revisions (Pull request #1725) @axel-lauer
- Wenzel16nature (Pull request #1692) @zechlau
- Add mask albedolandcover (Pull request #1673) @bascrezee
- IPCC AR5 fig. 9.3 (seasonality) (Pull request #1726) @axel-lauer
- Added additional emergent constraints on ECS (Pull request #1585) @schlunma
- A diagnostic to evaluate the turnover times of land ecosystem carbon (Pull request #1395) koir-su
- Removed multi\_model\_statistics step in recipe\_oceans\_example.yml as a workaround (Pull request #1779) @valeriupredoi

## 73.3 Documentation

- Extend getting started instructions to obtain config-user.yml (Pull request #1642) @Peter9192
- Extend information about native6 support on RTD (Pull request #1652) @Peter9192
- Update citation of ESMValTool paper in the doc (Pull request #1664) @mattiarighi
- Updated references to documentation (now docs.esmvaltool.org) (Pull request #1679) @axel-lauer
- Replace dead link with ESGF link. (Pull request #1681) @mattiarighi
- Add all European grants to Zenodo (Pull request #1682) @bouweandela
- Update Sphinx to v3 or later (Pull request #1685) @bouweandela
- Small fix to number of models in ensclus documentation (Pull request #1691) @jhardenberg
- Move draft\_release\_notes.py from ESMValCore to here and update (Pull request #1701) @bouweandela

- Improve the installation instructions (Pull request #1634) @valeriupredoi
- Improve description of how to implement provenance in diagnostic (Pull request #1750) @SarahAlidoost
- Update command line interface documentation and add links to ESMValCore configuration documentation (Pull request #1776) @bouweandela
- Documentation on how to find shapefiles for hydrology recipes (Pull request #1777) @JaroCamphuijsen

#### 73.4 Improvements

- Pin flake8<3.8.0 (Pull request #1635) @valeriupredoi
- Update conda package path in more places (Pull request #1636) @bouweandela
- Remove curly brackets around issue number in pull request template (Pull request #1637) @bouweandela
- Fix style issue in test (Pull request #1639) @bouweandela
- Update Codacy badges (Pull request #1662) @bouweandela
- Support extra installation methods in R (Pull request #1360) Javier Vegas-Regidor
- Add ncdf4.helpers package as a dependency again (Pull request #1678) @bouweandela
- Speed up conda installation (Pull request #1677) @bouweandela
- Update CMORizers and recipes for ESMValCore v2.0.0 (Pull request #1699) @SarahAlidoost
- Update setup.py for PyPI package (Pull request #1700) @bouweandela
- Cleanup recipe headers before the release (Pull request #1740) @mattiarighi
- Add colortables as esmvaltool subcommand (Pull request #1666) Javier Vegas-Regidor
- Increase version to v2.0.0 (Pull request #1756) @bouweandela
- Update job script (Pull request #1757) @mattiarighi
- Read authors and description from .zenodo.json (Pull request #1758) @bouweandela
- Update docker recipe to install from source (Pull request #1651) Javier Vegas-Regidor

#### 73.5 Observational and re-analysis dataset support

- Cmorize aphro ma (Pull request #1555) @mwjury
- Respectable testing for cmorizers/obs/utilities.py and cmorizers/obs/cmorize\_obs.py (Pull request #1517) @valeriupredoi
- Fix start year in recipe\_check\_obs (Pull request #1638) @mattiarighi
- Cmorizer for the PERSIANN-CDR precipitation data (Pull request #1633) @hb326
- Cmorize eobs (Pull request #1554) @mwjury
- Update download cds satellite lai fapar (Pull request #1654) @bascrezee
- Added monthly mean vars (ta, va, zg) to era5 cmorizer via recipe (Pull request #1644) @egalytska
- Make format time check more flexible (Pull request #1661) @mattiarighi
- Exclude od550lt1aer from recipe\_check\_obs.yml (Pull request #1720) @mattiarighi

- PERSIANN-CDR cmorizer update: adding the capability to save monthly mean files (Pull request #1728) @hb326
- Add standard\_name attribute to lon and lat in cmorize\_obs\_esacci\_oc.py (Pull request #1760) @tomaslovato
- Allow for incomplete months on daily frequency in cmorizer ncl utilities (Pull request #1754) @mattiarighi
- Fix AURA-TES cmorizer (Pull request #1766) @mattiarighi

#### CHAPTER

#### SEVENTYFOUR

#### V2.0.0B4

This release includes

#### 74.1 Bug fixes

- Fix HALOE plev coordinate (Pull request #1590) @mattiarighi
- Fix tro3 units in HALOE (Pull request #1591) @mattiarighi

#### 74.2 Diagnostics

- Applicate sea ice negative feedback (Pull request #1299) Javier Vegas-Regidor
- Add Russell18jgr ocean diagnostics (Pull request #1592) @bouweandela
- Refactor marrmot recipe and diagnostic to use ERA5 daily data made by new cmorizer (Pull request #1600) @SarahAlidoost
- In recipe\_wflow, use daily ERA5 data from the new cmorizer. (Pull request #1599) @Peter9192
- In wflow diagnostic, calculate PET after(!) interpolation and lapse rate correction (Pull request #1618) @jeromaerts
- Fixed wenz14jgr (Pull request #1562) @zechlau
- Update portrait\_plot.ncl (Pull request #1625) @bettina-gier

#### 74.3 Documentation

- Restructure documentation (Pull request #1587) @bouweandela
- Add more links to documentation (Pull request #1595) @bouweandela
- Update links in readme (Pull request #1598) @bouweandela
- Minor improvements to installation documentation (Pull request #1608) @bouweandela
- Add info for new mailing list to documentation. (Pull request #1607) @bjoernbroetz
- Update making a release documentation (Pull request #1627) @bouweandela

#### 74.4 Improvements

- Avoid broken pytest-html plugin (Pull request #1583) @bouweandela
- Remove reference section in config-references.yml (Pull request #1545) @SarahAlidoost
- Various improvements to development infrastructure (Pull request #1570) @bouweandela
- Install scikit-learn from conda, remove libunwind as a direct dependency (Pull request #1611) @valeriupredoi
- Create conda subpackages and enable tests (Pull request #1624) @bouweandela

## 74.5 Observational and re-analysis dataset support

- Cmorizer for HALOE (Pull request #1581) @mattiarighi
- Add CMORizer for CT2019 (Pull request #1604) @schlunma

For older releases, see the release notes on https://github.com/ESMValGroup/ESMValTool/releases.

## Part XIII

# **Indices and tables**

- genindex
- search

#### **PYTHON MODULE INDEX**

е esmvaltool.diag\_scripts.mlr.models.svr, 823 esmvaltool.diag\_scripts.emergent\_constraints, esmvaltool.diag\_scripts.mlr.plot,651 esmvaltool.diag\_scripts.mlr.postprocess, 653 639 esmvaltool.diag\_scripts.emergent\_constraints.cox18nature; diag\_scripts.mlr.preprocess, 655 esmvaltool.diag\_scripts.mlr.rescale\_with\_emergent\_constrained 635 esmvaltool.diag\_scripts.emergent\_constraints.ecs\_scatter, esmvaltool.diag\_scripts.monitor.compute\_eofs, 636 esmvaltool.diag\_scripts.emergent\_constraints.multiple\_constraints, esmvaltool.diag\_scripts.monitor.monitor, 832 637 esmvaltool.diag\_scripts.emergent\_constraints.simyle\_toolstdiag.tscripts.monitor.monitor\_base, 844 638 esmvaltool.diag\_scripts.monitor.multi\_datasets, esmvaltool.diag\_scripts.mlr,658 835 esmvaltool.diag\_scripts.mlr.custom\_sklearn, esmvaltool.diag\_scripts.ocean.diagnostic\_maps, 664 846 esmvaltool.diag\_scripts.mlr.evaluate\_residuals, esmvaltool.diag\_scripts.ocean.diagnostic\_maps\_quad, 648 847 esmvaltool.diag\_scripts.mlr.main, 649 esmvaltool.diag\_scripts.ocean.diagnostic\_model\_vs\_obs, esmvaltool.diag\_scripts.mlr.mmm, 650 849 esmvaltool.diag\_scripts.mlr.models, 689 esmvaltool.diag\_scripts.ocean.diagnostic\_profiles, esmvaltool.diag\_scripts.mlr.models.gbr\_base, 851 703 esmvaltool.diag\_scripts.mlr.models.gbr\_sklearnesmvaltool.diag\_scripts.ocean.diagnostic\_seaice, 858 719 esmvaltool.diag\_scripts.mlr.models.gbr\_xgboost<sup>esmvaltool.diag\_scripts.ocean.diagnostic\_timeseries,</sup> 853 728 esmvaltool.diag\_scripts.mlr.models.gpr\_sklearnesmvaltool.diag\_scripts.ocean.diagnostic\_tools, 861 736 esmvaltool.diag\_scripts.ocean.diagnostic\_transects, esmvaltool.diag\_scripts.mlr.models.huber,749 855 esmvaltool.diag\_scripts.mlr.models.krr,757 esmvaltool.diag\_scripts.psyplot\_diag, 867 esmvaltool.diag\_scripts.mlr.models.lasso,765 esmvaltool.diag\_scripts.seaborn\_diag, 867 esmvaltool.diag\_scripts.mlr.models.lasso\_cv, esmvaltool.diag\_scripts.shared, 615 773 esmvaltool.diag\_scripts.mlr.models.lasso\_lars\_esmvaltool.diag\_scripts.shared.iris\_helpers, 628 781 esmvaltool.diag\_scripts.shared.plot, 631 esmvaltool.diag\_scripts.mlr.models.linear, 790 esmvaltool.diag\_scripts.mlr.models.linear\_base, 711 esmvaltool.diag\_scripts.mlr.models.rfr,798 esmvaltool.diag\_scripts.mlr.models.ridge, 807 esmvaltool.diag\_scripts.mlr.models.ridge\_cv, 815

## INDEX

## Α

add_dataset() (4	esmval-	bgc_uni	ts()	(in	module	esmval-
tool.diag_scripts.shared.Datasets m 616	iethod),		tool.diag_ 862	scripts.oce	an.diagnostic_to	pols),
add_legend_outside_right() (in module tool.diag_scripts.ocean.diagnostic_tool		С				
add_linear_regression() (in module tool.diag_scripts.ocean.diagnostic_mod 849					.es() (in moa ocean.diagnostic	
add_map_subplot() (in module	esmval-	categor	ical_feat	tures		(esmval-
tool.diag_scripts.ocean.diagnostic_map 848	os_quad),		tool.diag_ property),	-	models.gbr_bas	e.GBRModel
			ical_feat	tures		(esmval-
tool.diag_scripts.ocean.diagnostic_mod 850	lel_vs_obs	s),	tool.diag_ property),	-	models.gbr_skle	earn.SklearnGBRModel
		categor	ical_feat			(esmval-
tool.diag_scripts.ocean.diagnostic_tran. 855			tool.diag_ property),	-	models.gbr_xgb	oost.XGBoostGBRModel
		categor	ical_feat			(esmval-
tool.diag_scripts.shared.Datasets m 616	iethod),		tool.diag_ property),	-	models.gpr_skle	earn.SklearnGPRModel
<pre>add_vars() (esmvaltool.diag_scripts.shared.Va</pre>	ariables	categor	ical_feat	tures		(esmval-
method), 622			tool.diag_	scripts.mlr.	models.huber.H	uberRegressionModel
AdvancedGaussianProcessRegressor (class			property),			
valtool.diag_scripts.mlr.models.gpr_skl	earn),	categor	ical_feat			(esmval-
736 AdvancedPipeline ( <i>class in</i>	annal		-	-	models.krr.KRR	Model
AdvancedPipeline (class in tool.diag_scripts.mlr.custom_sklearn), 6	esmval- 564	catagor	<pre>property), ical_feat</pre>			(esmval-
	esmval-	categoi			models.lasso.La	
tool.diag_scripts.mlr.custom_sklearn), 6			property),		moueis.iusso.Lu	5501110aei
	esmval-	categor	ical_feat			(esmval-
tool.diag_scripts.mlr.custom_sklearn), 6	578				models.lasso cv	.LassoCVModel
AdvancedTransformedTargetRegressor (cl	ass in		property),	· ·	_	
esmvaltool.diag_scripts.mlr.custom_skle	earn),		ical_feat			(esmval-
683			tool.diag_	scripts.mlr.	models.lasso_la	rs_cv.LassoLarsCVModel
	esmval-		property),			
tool.diag_scripts.ocean.diagnostic_seai	ce),	categor	ical_feat			(esmval-
859	_				models.linear.Li	inearRegressionModel
	esmval-		property),			
tool.diag_scripts.shared), 624		categor	ical_feat			(esmval-
			tool.diag property),		models.linear_b	ase.LinearModel
			· · · //			

В

tool.diag_scripts.mlr.models.MLRModel	<pre>create() (esmvaltool.diag_scripts.mlr.models.krr.KRRModel</pre>
property), 696 categorical_features (esmval-	<pre>create() (esmvaltool.diag_scripts.mlr.models.lasso.LassoModel</pre>
tool.diag_scripts.mlr.models.rfr.RFRModel property), 800	<pre>create() (esmvaltool.diag_scripts.mlr.models.lasso_cv.LassoCVModel</pre>
categorical_features (esmval-	create() (esmvaltool.diag_scripts.mlr.models.lasso_lars_cv.LassoLarsCV.
tool.diag_scripts.mlr.models.ridge.RidgeModel	class method), 783
property), 808	$\verb create()  (esmval to ol. diag\_scripts.mlr.models.linear.LinearRegressionModels.linear.LinearRegressionRegressionRegressionRegressionRegressionRegressionRegressionRegressionRegressionRegressionRegressioRegressioRe$
categorical_features (esmval-	class method), 792
	(adeeate() (esmvaltool.diag_scripts.mlr.models.linear_base.LinearModel
property), 816	class method), 712
categorical_features (esmval- tool.diag_scripts.mlr.models.svr.SVRModel	<pre>create() (esmvaltool.diag_scripts.mlr.models.MLRModel</pre>
property), 825	create() (esmvaltool.diag_scripts.mlr.models.rfr.RFRModel
cdf() (in module esmval-	class method), 800
tool.diag_scripts.emergent_constraints),	<pre>create() (esmvaltool.diag_scripts.mlr.models.ridge.RidgeModel</pre>
640 check_coordinate() (in module esmval-	class method), 808
tool.diag_scripts.shared.iris_helpers), 628	<pre>create() (esmvaltool.diag_scripts.mlr.models.ridge_cv.RidgeCVModel</pre>
<pre>check_metadata() (in module esmval- tool.diag_scripts.emergent_constraints),</pre>	<pre>create() (esmvaltool.diag_scripts.mlr.models.svr.SVRModel</pre>
640	create_alias() (in module esmval-
<pre>check_predict_kwargs() (in module esmval-</pre>	tool.diag_scripts.mlr), 658
tool.diag_scripts.mlr), 658	create_ice_cmap() (in module esmval-
classes_(esmvaltool.diag_scripts.mlr.custom_sklearn.Ad property), 665	vancedPip <b>eliak</b> diag_scripts.ocean.diagnostic_seaice), 859
classes_(esmvaltool.diag_scripts.mlr.custom_sklearn.Ad	
property), 673	tool.diag_scripts.emergent_constraints), 641
classes_(esmvaltool.diag_scripts.mlr.custom_sklearn.Ad	
property), 678	tool.diag_scripts.mlr.custom_sklearn), 689
<pre>coef_(esmvaltool.diag_scripts.mlr.custom_sklearn.Advand property), 665</pre>	c <b>eduBip_etiimae_to_float()</b> (in module esmval- tool.diag_scripts.ocean.diagnostic_tools),
coef_(esmvaltool.diag_scripts.mlr.custom_sklearn.Advand	
property), 683	D
combine_groups() (in module esmval-	
<i>tool.diag_scripts.emergent_constraints</i> ), 641	<pre>data(esmvaltool.diag_scripts.mlr.models.gbr_base.GBRModel</pre>
constraint_info_array() (in module esmval-	data (esmvaltool.diag_scripts.mlr.models.gbr_sklearn.SklearnGBRModel
tool.diag_scripts.emergent_constraints), 641	property), 721
convert_to_iris() (in module esmval-	data (esmvaltool.diag_scripts.mlr.models.gbr_xgboost.XGBoostGBRModel
tool.diag_scripts.shared.iris_helpers), 629	property), 729
count() (esmvaltool.diag_scripts.shared.Variable method), 621	<pre>data(esmvaltool.diag_scripts.mlr.models.gpr_sklearn.SklearnGPRModel</pre>
	BBMo(ks/mvaltool.diag_scripts.mlr.models.huber.HuberRegressionModel
class method), 704	property), 750
<pre>create() (esmvaltool.diag_scripts.mlr.models.gbr_sklearn</pre>	n <b>dåtea(vsinkklunde</b> liag_scripts.mlr.models.krr.KRRModel property), 759
<pre>create() (esmvaltool.diag_scripts.mlr.models.gbr_xgboos</pre>	stoXGB(costfGBRMhdidg_scripts.mlr.models.lasso.LassoModel property), 766
	nSitea(winRibodeliag_scripts.mlr.models.lasso_cv.LassoCVModel
class method), 742	property), 775
	property, repaired and the second state of the
class method), 750	property), 783

#### ESMValTool User's and Developer's Guide, Release 2.11.0.dev52+g696097c.d20240424

data (esmvaltool.diag_scripts.r property), 792	mlr.models.linear.LinearReg	r <b>e£sionMo(desi</b> mvaltool.diag_scripts.mlr.models.lasso_cv.LassoCVModel method), 775
1 1 2	mlrmodels linear base Line	ca <b>stex</b> (Q) (esmvaltool.diag_scripts.mlr.models.lasso_lars_cv.LassoLarsCVM
property), 712	nii.moueis.ineur_buse.Line	method), 783
data (esmvaltool.diag_scrip	pts.mlr.models.MLRModel	efecv() (esmvaltool.diag_scripts.mlr.models.linear.LinearRegressionModels.
property), 696		<i>method</i> ), 792
	.mlr.models.rfr.RFRModel	efecv() (esmvaltool.diag_scripts.mlr.models.linear_base.LinearModel
property), 800		<i>method</i> ), 712
data (esmvaltool.diag_scripts.r property), 808	nlr.models.ridge.RidgeMode	<pre>ekfecv() (esmvaltool.diag_scripts.mlr.models.MLRModel</pre>
data(esmvaltool.diag_scripts.	mlr.models.ridge_cv.RidgeC	VeMedvl() (esmvaltool.diag_scripts.mlr.models.rfr.RFRModel
property), 817		<i>method</i> ), 800
	.mlr.models.svr.SVRModel	efecv() (esmvaltool.diag_scripts.mlr.models.ridge.RidgeModel
property), 825		method), 808
Datasets (class in esmvaltool.		efecv() (esmvaltool.diag_scripts.mlr.models.ridge_cv.RidgeCVModel
datasets_have_mlr_attrib		method), 817
valtool.diag_scripts.r		efecv() (esmvaltool.diag_scripts.mlr.models.svr.SVRModel
<pre>decadal_average() (in</pre>		method), 825
tool.diag_scripts.oce 863	an.alagnostic_tools),	<pre>esmvaltool.diag_scripts.emergent_constraints   module, 639</pre>
decision_function()	(agrand	esmvaltool.diag_scripts.emergent_constraints.cox18nature
	.custom_sklearn.AdvancedPi	
method), 665	cusiom_skieurn.Auvanceur	esmvaltool.diag_scripts.emergent_constraints.ecs_scatter
decision_function()	(esmval-	module, 636
		Resmvaltool.diag_scripts.emergent_constraints.multiple_constraints.multi
method), 673	eusiom_smearm.ravanceard	module, 637
<pre>decision_function()</pre>	(esmval-	esmvaltool.diag_scripts.emergent_constraints.single_constr
	custom_sklearn.AdvancedR	
method), 678	—	esmvaltool.diag_scripts.mlr
<pre>determine_profiles_str()</pre>	(in module esmval-	module, 658
tool.diag_scripts.oce	an.diagnostic_profiles),	esmvaltool.diag_scripts.mlr.custom_sklearn
852		module, 664
<pre>determine_set_y_logscale</pre>	() (in module esmval-	<pre>esmvaltool.diag_scripts.mlr.evaluate_residuals</pre>
tool.diag_scripts.oce	an.diagnostic_transects),	module, 648
856		esmvaltool.diag_scripts.mlr.main
<pre>determine_transect_str()</pre>		module, 649
0— I	an.diagnostic_transects),	esmvaltool.diag_scripts.mlr.mmm
856		module, 650
E		esmvaltool.diag_scripts.mlr.models
		module, 689
	pts.mlr.models.gbr_base.GB	<pre>ReMoveltool.diag_scripts.mlr.models.gbr_base</pre>
method), 704		module, 703
	pts.mtr.models.gbr_sklearn.	<pre>SktenwaltBRM.ddcag_scripts.mlr.models.gbr_sklearn module, 719</pre>
<i>method</i> ), 721	interminimedale abre vaboost	.XSBV@1KGBRMideg_scripts.mlr.models.gbr_xgboost
method), 729	pis.mir.models.gor_xgooosi.	module, 728
	ints mlr models anr sklearn	StanwaltBRM dddg_scripts.mlr.models.gpr_sklearn
method), 742	pis.mir.modeis.gpr_skiedrii.	module, 736
	pts.mlr.models.huber.Huber	Regnoslandbddiag_scripts.mlr.models.huber
<i>method</i> ), 750		module, 749
	pts.mlr.models.krr.KRRMod	d∉smvaltool.diag_scripts.mlr.models.krr
<i>method</i> ), 759	_	module, 757
	pts.mlr.models.lasso.LassoN	/@gmValtool.diag_scripts.mlr.models.lasso
<i>method</i> ), 766		module, 765

esmvaltool.diag\_scripts.mlr.models.lasso\_cv esmvaltool.diag\_scripts.shared.iris\_helpers module.773 module. 628 esmvaltool.diag\_scripts.mlr.models.lasso\_lars\_esmvaltool.diag\_scripts.shared.plot module, 631 module, 781 esmvaltool.diag\_scripts.mlr.models.linear export\_csv() (in module esmvalmodule, 790 tool.diag scripts.emergent constraints), esmvaltool.diag\_scripts.mlr.models.linear\_base 642 module, 711 export\_prediction\_data() (esmvalesmvaltool.diag\_scripts.mlr.models.rfr tool.diag\_scripts.mlr.models.gbr\_base.GBRModel module, 798 method), 705 esmvaltool.diag\_scripts.mlr.models.ridge export\_prediction\_data() (esmvaltool.diag\_scripts.mlr.models.gbr\_sklearn.SklearnGBRModel module, 807 esmvaltool.diag\_scripts.mlr.models.ridge\_cv method), 721 module, 815 export\_prediction\_data() (esmvalesmvaltool.diag\_scripts.mlr.models.svr tool.diag\_scripts.mlr.models.gbr\_xgboost.XGBoostGBRModel method), 730 module, 823 esmvaltool.diag\_scripts.mlr.plot export\_prediction\_data() (esmvalmodule, 651 tool.diag\_scripts.mlr.models.gpr\_sklearn.SklearnGPRModel esmvaltool.diag\_scripts.mlr.postprocess method), 743 module. 653 export\_prediction\_data() (esmvalesmvaltool.diag\_scripts.mlr.preprocess tool.diag\_scripts.mlr.models.huber.HuberRegressionModel module, 655 method), 751 esmvaltool.diag\_scripts.mlr.rescale\_with\_emergentorconstantion\_data() (esmvalmodule. 657 tool.diag scripts.mlr.models.krr.KRRModel esmvaltool.diag\_scripts.monitor.compute\_eofs method), 759 module.834 export\_prediction\_data() (esmvalesmvaltool.diag\_scripts.monitor.monitor tool.diag\_scripts.mlr.models.lasso.LassoModel module, 832 method), 767 esmvaltool.diag\_scripts.monitor.monitor\_base export\_prediction\_data() (esmvaltool.diag\_scripts.mlr.models.lasso\_cv.LassoCVModel module. 844 esmvaltool.diag\_scripts.monitor.multi\_datasets method), 775 module, 835 export\_prediction\_data() (esmvalesmvaltool.diag\_scripts.ocean.diagnostic\_maps tool.diag\_scripts.mlr.models.lasso\_lars\_cv.LassoLarsCVModel module, 846 method), 784 esmvaltool.diag\_scripts.ocean.diagnostic\_maps\_expandrt\_prediction\_data() (esmvaltool.diag\_scripts.mlr.models.linear.LinearRegressionModel module.847 esmvaltool.diag\_scripts.ocean.diagnostic\_model\_vs\_obs method), 792 module, 848 export\_prediction\_data() (esmvalesmvaltool.diag\_scripts.ocean.diagnostic\_profiles tool.diag\_scripts.mlr.models.linear\_base.LinearModel module, 851 method), 713 esmvaltool.diag\_scripts.ocean.diagnostic\_seaicexport\_prediction\_data() (esmvalmodule, 857 tool.diag scripts.mlr.models.MLRModel esmvaltool.diag\_scripts.ocean.diagnostic\_timeseries method), 696 module, 853 export\_prediction\_data() (esmvalesmvaltool.diag\_scripts.ocean.diagnostic\_tools tool.diag\_scripts.mlr.models.rfr.RFRModel method), 800 module, 861 esmvaltool.diag\_scripts.ocean.diagnostic\_transecqtosrt\_prediction\_data() (esmvalmodule, 855 tool.diag\_scripts.mlr.models.ridge.RidgeModel esmvaltool.diag\_scripts.psyplot\_diag method), 809 module, 867 export\_prediction\_data() (esmvalesmvaltool.diag\_scripts.seaborn\_diag tool.diag\_scripts.mlr.models.ridge\_cv.RidgeCVModel module, 867 method), 817 esmvaltool.diag\_scripts.shared export\_prediction\_data() (esmvalmodule, 615 tool.diag scripts.mlr.models.svr.SVRModel

<i>method</i> ), 825	tool.diag_scripts.mlr.custom_sklearn.AdvancedPipeline
export_training_data() (esmval-	
tool.diag_scripts.mlr.models.gbr_base.GBRMod	
method), 705	tool.diag_scripts.mlr.custom_sklearn.AdvancedTransformedTarge
export_training_data() (esmval-	property), 683
tool.diag_scripts.mlr.models.gbr_sklearn.Sklea	rn <b>GBRWand</b> elnames_in_ (esmval-
<i>method</i> ), 721	tool.diag_scripts.mlr.custom_sklearn.AdvancedPipeline
export_training_data() (esmval-	1 1 577
tool.diag_scripts.mlr.models.gbr_xgboost.XGB6 method), 730	pos <b>fGBRMosl</b> (ksmvaltool.diag_scripts.mlr.models.gbr_base.GBRModel property), 705
	features (esmvaltool.diag_scripts.mlr.models.gbr_sklearn.SklearnGBRM
tool.diag_scripts.mlr.models.gpr_sklearn.Sklear	
method), 743	features (esmvaltool.diag_scripts.mlr.models.gbr_xgboost.XGBoostGBRI
export_training_data() (esmval-	
	ssi <b>beMaded</b> s (esmvaltool.diag_scripts.mlr.models.gpr_sklearn.SklearnGPRM
method), 751	property), 743
<pre>export_training_data() (esmval-</pre>	
tool.diag_scripts.mlr.models.krr.KRRModel	property), 751
<i>method</i> ), 759	<pre>features(esmvaltool.diag_scripts.mlr.models.krr.KRRModel</pre>
export_training_data() (esmval-	
	<pre>features(esmvaltool.diag_scripts.mlr.models.lasso.LassoModel</pre>
<i>method</i> ), 767	property), 767
	features (esmvaltool.diag_scripts.mlr.models.lasso_cv.LassoCVModel
tool.diag_scripts.mlr.models.lasso_cv.LassoCV	
<i>method</i> ), 775	features (esmvaltool.diag_scripts.mlr.models.lasso_lars_cv.LassoLarsCV
export_training_data() (esmval-	
	colfarsCWWesdelsmvaltool.diag_scripts.mlr.models.linear.LinearRegressionMod
method), 784	property), 792
<pre>export_training_data() (esmval- tool.diag_scripts.mlr.models.linear.LinearRegree</pre>	features (esmvaltool.diag_scripts.mlr.models.linear_base.LinearModel
method), 792	features (esmvaltool.diag_scripts.mlr.models.MLRModel
export_training_data() (esmval-	
	rM <b>beat</b> ures (esmvaltool.diag_scripts.mlr.models.rfr.RFRModel
method), 713	property), 801
export_training_data() (esmval-	
tool.diag_scripts.mlr.models.MLRModel	property), 809
<i>method</i> ), 697	<pre>features(esmvaltool.diag_scripts.mlr.models.ridge_cv.RidgeCVModel</pre>
<pre>export_training_data() (esmval-</pre>	property), 817
tool.diag_scripts.mlr.models.rfr.RFRModel	<pre>features(esmvaltool.diag_scripts.mlr.models.svr.SVRModel</pre>
<i>method</i> ), 801	property), 826
export_training_data() (esmval-	
tool.diag_scripts.mlr.models.ridge.RidgeModel	tool.diag_scripts.mlr.models.gbr_base.GBRModel
method), 809	property), 705
export_training_data() (esmval-	
tool.diag_scripts.mlr.models.ridge_cv.RidgeCV method), 817	
export_training_data() (esmval-	property), 721 features_after_preprocessing (esmval-
tool.diag_scripts.mlr.models.svr.SVRModel	tool.diag_scripts.mlr.models.gbr_xgboost.XGBoostGBRModel
method), 826	property), 730
extract_variables() (in module esmval-	
tool.diag_scripts.shared), 625	tool.diag_scripts.mlr.models.gpr_sklearn.SklearnGPRModel
	property), 743
F	features_after_preprocessing (esmval-
feature_importances_ (esmval-	
	*

property), 751	property), 767
features_after_preprocessing (esmval-	
tool.diag_scripts.mlr.models.krr.KRRModel	tool.diag_scripts.mlr.models.lasso_cv.LassoCVModel
property), 759	property), 775
features_after_preprocessing (esmval-	
tool.diag_scripts.mlr.models.lasso.LassoModel	tool.diag_scripts.mlr.models.lasso_lars_cv.LassoLarsCVModel
property), 767	property), 784
features_after_preprocessing (esmval-	features_types (esmval-
tool.diag_scripts.mlr.models.lasso_cv.LassoCVM	lodel tool.diag_scripts.mlr.models.linear.LinearRegressionModel
property), 775	property), 792
features_after_preprocessing (esmval-	
	bLarsCVMo <b>tba</b> ll.diag_scripts.mlr.models.linear_base.LinearModel
property), 784	property), 713
	features_types (esmval-
	sionModel tool.diag_scripts.mlr.models.MLRModel
property), 792	property), 697
features_after_preprocessing (esmval-	
tool.diag_scripts.mlr.models.linear_base.Linear	
property), 713	property), 801
features_after_preprocessing (esmval-	
tool.diag_scripts.mlr.models.MLRModel	tool.diag_scripts.mlr.models.ridge.RidgeModel
property), 697	property), 809
features_after_preprocessing (esmval-	features_types (esmval- tool.diag_scripts.mlr.models.ridge_cv.RidgeCVModel
tool.diag_scripts.mlr.models.rfr.RFRModel property), 801	property), 817
features_after_preprocessing (esmval-	
tool.diag_scripts.mlr.models.ridge.RidgeModel	tool.diag_scripts.mlr.models.svr.SVRModel
property), 809	property), 826
features_after_preprocessing (esmval-	
tool.diag_scripts.mlr.models.ridge_cv.RidgeCVM	
property), 817	property), 705
features_after_preprocessing (esmval-	
tool.diag_scripts.mlr.models.svr.SVRModel	tool.diag_scripts.mlr.models.gbr_sklearn.SklearnGBRModel
property), 826	property), 721
	features_units (esmval-
tool.diag_scripts.mlr.models.gbr_base.GBRMode	el tool.diag_scripts.mlr.models.gbr_xgboost.XGBoostGBRModel
property), 705	property), 730
features_types (esmval-	features_units (esmval-
tool.diag_scripts.mlr.models.gbr_sklearn.Sklearn	1GBRModelool.diag_scripts.mlr.models.gpr_sklearn.SklearnGPRModel
property), 721	property), 743
	features_units (esmval-
	ostGBRModøbl.diag_scripts.mlr.models.huber.HuberRegressionModel
property), 730	property), 751
	features_units (esmval-
· · · · · ·	1GPRModelool.diag_scripts.mlr.models.krr.KRRModel
property), 743	property), 759
	features_units (esmval-
· · · ·	sionModel tool.diag_scripts.mlr.models.lasso.LassoModel
property), 751	property), 767
features_types (esmval-	features_units (esmval-
tool.diag_scripts.mlr.models.krr.KRRModel	tool.diag_scripts.mlr.models.lasso_cv.LassoCVModel
property), 759	property), 775
features_types (esmval-	features_units (esmval- tool diag. scripts mlr models lasso lars cy Lasso Lars CVM odel
tool.diag_scripts.mlr.models.lasso.LassoModel	tool.diag_scripts.mlr.models.lasso_lars_cv.LassoLarsCVModel

704	(i+() ( and the state of the st
property), 784 features_units (esmval-	<pre>fit() (esmvaltool.diag_scripts.mlr.models.linear.LinearRegressionModel</pre>
	ssfintMJdesmvaltool.diag_scripts.mlr.models.linear_base.LinearModel
property), 792	method), 713
features_units (esmval-	$\mathbf{c} = 1$
tool.diag_scripts.mlr.models.linear_base.Linear	
property), 713	<pre>fit() (esmvaltool.diag_scripts.mlr.models.rfr.RFRModel</pre>
features_units (esmval-	<i>method</i> ), 801
tool.diag_scripts.mlr.models.MLRModel	fit() (esmvaltool.diag_scripts.mlr.models.ridge.RidgeModel
property), 697	method), 809
features_units (esmval-	<pre>fit() (esmvaltool.diag_scripts.mlr.models.ridge_cv.RidgeCVModel</pre>
tool.diag_scripts.mlr.models.rfr.RFRModel	method), 817
property), 801 features_units (esmval-	<pre>fit() (esmvaltool.diag_scripts.mlr.models.svr.SVRModel</pre>
tool.diag_scripts.mlr.models.ridge.RidgeModel	fit_kwargs (esmvaltool.diag_scripts.mlr.models.gbr_base.GBRModel
property), 809	property), 705
features_units (esmval-	fit_kwargs (esmvaltool.diag_scripts.mlr.models.gbr_sklearn.SklearnGBR
tool.diag_scripts.mlr.models.ridge_cv.RidgeCVM	
<i>property</i> ), 817	fit_kwargs (esmvaltool.diag_scripts.mlr.models.gbr_xgboost.XGBoostGB
features_units (esmval-	<i>property</i> ), 730
tool.diag_scripts.mlr.models.svr.SVRModel	fit_kwargs(esmvaltool.diag_scripts.mlr.models.gpr_sklearn.SklearnGPR
property), 826	property), 743
FeatureSelectionTransformer (class in esmval-	<pre>fit_kwargs(esmvaltool.diag_scripts.mlr.models.huber.HuberRegressionM</pre>
tool.diag_scripts.mlr.custom_sklearn), 686	property), 751
	c&dRipkeWavegs(esmvaltool.diag_scripts.mlr.models.krr.KRRModel
<i>method</i> ), 665	property), 760
	cddREEwargs (esmvaltool.diag_scripts.mlr.models.lasso.LassoModel
method), 673	property), 767
method), 678	cddREE664rgs (esmvaltool.diag_scripts.mlr.models.lasso_cv.LassoCVModel property), 776
	c <b>&amp;dTir_kwfargze</b> (kKungalRugledisagr_scripts.mlr.models.lasso_lars_cv.LassoLars
method), 683	property), 784
	efile_kwafgsw.commaltool.diag_scripts.mlr.models.linear.LinearRegressionN
<i>method</i> ), 687	property), 793
<pre>fit() (esmvaltool.diag_scripts.mlr.models.gbr_base.GBR</pre>	Mfidelkwargs (esmvaltool.diag_scripts.mlr.models.linear_base.LinearModel
<i>method</i> ), 705	property), 713
	le <b>firn_(KBillMyBl</b> edsmvaltool.diag_scripts.mlr.models.MLRModel
<i>method</i> ), 721	property), 697
	GBioosKiBRoscashvaltool.diag_scripts.mlr.models.rfr.RFRModel
method), 730	property), 801
	lvfintel@angsi@esfmoaltxxRediregsorripts.mlr.models.ridge.RidgeModel
method), 737	property), 809 le <b>firn<u>(</u>RRBMps</b> )edsmvaltool.diag_scripts.mlr.models.ridge_cv.RidgeCVModel
method), 743	property), 818
	gfassidswarogs((esmvaltool.diag_scripts.mlr.models.svr.SVRModel
method), 751	property), 826
fit() (esmvaltool.diag_scripts.mlr.models.krr.KRRModel	
method), 759	tool.diag_scripts.mlr.custom_sklearn.AdvancedPipeline
fit() (esmvaltool.diag_scripts.mlr.models.lasso.LassoMo	
<i>method</i> ), 767	<pre>fit_target_transformer_only() (esmval-</pre>
<pre>fit() (esmvaltool.diag_scripts.mlr.models.lasso_cv.Lasso</pre>	CVModel tool.diag_scripts.mlr.custom_sklearn.AdvancedPipeline
method), 775	<i>method</i> ), 666
<pre>fit() (esmvaltool.diag_scripts.mlr.models.lasso_lars_cv.l</pre>	
method), 784	$tool.diag\_scripts.mlr.custom\_sklearn.AdvancedPipeline$

<i>method</i> ), 667			<i>method</i> ), 776	
<pre>fit_transform()</pre>	(esmval-	get_anc	estors()	(esmval-
tool.diag_scripts.mlr.custom_sklearn.	AdvancedR	FE	tool.diag_scripts.mlr.models.lasso_l	lars_cv.LassoLarsCVModel
<i>method</i> ), 673			<i>method</i> ), 784	
<pre>fit_transform()</pre>	(esmval-	get_anc	estors()	(esmval-
tool.diag_scripts.mlr.custom_sklearn.	AdvancedR	FECV	tool.diag_scripts.mlr.models.linear.	LinearRegressionModel
method), 678			method), 793	-
<pre>fit_transform()</pre>	(esmval-	get_anc	estors()	(esmval-
tool.diag_scripts.mlr.custom_sklearn.	FeatureSele	ectionTran.	s <b>formhdi</b> ag_scripts.mlr.models.linear_	_base.LinearModel
method), 687			method), 713	
<pre>fit_transformer_only()</pre>	(esmval-	get_anc	estors()	(esmval-
tool.diag_scripts.mlr.custom_sklearn.	AdvancedT	ransformed	dífærðg <b>diRggsessipt</b> s.mlr.models.MLRM	lodel
method), 683			<i>method</i> ), 697	
<pre>fit_transformers_only()</pre>	(esmval-	get_anc	estors()	(esmval-
tool.diag_scripts.mlr.custom_sklearn.	AdvancedP	ipeline	tool.diag_scripts.mlr.models.rfr.RFI	RModel
method), 667		-	<i>method</i> ), 801	
folder() (in module	esmval-	get_anc	estors()	(esmval-
tool.diag_scripts.ocean.diagnostic_to	ols),		tool.diag_scripts.mlr.models.ridge.k	RidgeModel
863			<i>method</i> ), 809	
0		get_anc	estors()	(esmval-
G			tool.diag_scripts.mlr.models.ridge_o	cv.RidgeCVModel
GBRModel (class in	esmval-		<i>method</i> ), 818	
tool.diag_scripts.mlr.models.gbr_base	e), 703	get_anc	estors()	(esmval-
get_1d_cube() (in module	esmval-		tool.diag_scripts.mlr.models.svr.SVI	RModel
tool.diag_scripts.mlr), 659			<i>method</i> ), 826	
<pre>get_absolute_time_units() (in module</pre>	esmval-	get_are	a_weights() (in module	esmval-
tool.diag_scripts.mlr), 659			tool.diag_scripts.mlr), 660	
<pre>get_alias() (in module esmvaltool.diag_sch</pre>	ripts.mlr),	get_arr		esmval-
660			tool.diag_scripts.ocean.diagnostic_	tools),
<pre>get_all_weights() (in module</pre>	esmval-		863	
tool.diag_scripts.mlr), 660		get_cap	tion() (in module	esmval-
<pre>get_ancestors()</pre>	(esmval-		tool.diag_scripts.emergent_constrai	ints),
tool.diag_scripts.mlr.models.gbr_base	e.GBRMode		642	
<i>method</i> ), 705		get_cfg	() (in module esmvaltool.diag_scrip	pts.shared),
<pre>get_ancestors()</pre>	(esmval-		625	
tool.diag_scripts.mlr.models.gbr_skle	arn.Sklearn	I <b>GBRM0</b> Å		esmval-
<i>method</i> ), 722			tool.diag_scripts.emergent_constrai	nts),
get_ancestors()	(esmval-	_	642	_
tool.diag_scripts.mlr.models.gbr_xgb	oost.XGBoo	geBRMb		
<i>method</i> ), 730			tool.diag_scripts.ocean.diagnostic_	tools),
get_ancestors()	(esmval-		863	
tool.diag_scripts.mlr.models.gpr_skle	arn.Sklearn	IGPRMOD		esmval-
<i>method</i> ), 743			tool.diag_scripts.emergent_constrai	nts),
get_ancestors()	(esmval-		643	
tool.diag_scripts.mlr.models.huber.Hi	uberRegress	siØAMAAI		
<i>method</i> ), 751			tool.diag_scripts.emergent_constrai	
get_ancestors()	(esmval-	get_con	trol_exper_obs() (in module	e esmval-
tool.diag_scripts.mlr.models.krr.KRR	Model		tool.diag_scripts.shared), 625	7
method), 760	, -	get_cub	e_range() (in module	esmval-
get_ancestors()	(esmval-		tool.diag_scripts.ocean.diagnostic_	tools),
tool.diag_scripts.mlr.models.lasso.La.	ssoModel		864	7
method), 767	, .	get_cub	e_range_diff() (in module	
get_ancestors()	(esmval-		tool.diag_scripts.ocean.diagnostic_	tools),
tool.diag_scripts.mlr.models.lasso_cv	.LassoCVM	odel	864	

<pre>get_data() (esmvaltool.diag_scripts.share</pre>		tool.diag_scripts.shared.Datasets method), 617
<pre>get_data_frame()</pre>	(esmval-	<pre>get_dataset_info_list() (esmval-</pre>
tool.diag_scripts.mlr.models.gbr_ba method), 706	se.GBRMode	lel tool.diag_scripts.shared.Datasets method), 618
get_data_frame()	(esmval-	get_dataset_style() (in module esmval-
tool.diag_scripts.mlr.models.gbr_skl		nGBRModelool.diag_scripts.shared.plot), 631
method), 722		get_decade() (in module esmval-
get_data_frame()	(esmval-	tool.diag_scripts.ocean.diagnostic_tools),
tool.diag_scripts.mlr.models.gbr_xgl		
<i>method</i> ), 731		<pre>get_diagnostic_filename() (in module esmval-</pre>
<pre>get_data_frame()</pre>	(esmval-	tool.diag_scripts.shared), 625
tool.diag_scripts.mlr.models.gpr_skl		
method), 744	etti monetti i	tool.diag_scripts.mlr.custom_sklearn.AdvancedPipeline
<pre>get_data_frame()</pre>	(esmval-	method), 667
tool.diag_scripts.mlr.models.huber.H		
method), 752	indernegress	tool.diag_scripts.mlr.custom_sklearn.AdvancedRFE
get_data_frame()	(esmval-	
tool.diag_scripts.mlr.models.krr.KRF		
method), 760	Mouer	tool.diag_scripts.mlr.custom_sklearn.AdvancedRFECV
get_data_frame()	(asmual	
-	(esmval-	
tool.diag_scripts.mlr.models.lasso.La	ussomoaei	
method), 768	(1	tool.diag_scripts.mlr.custom_sklearn.FeatureSelectionTransforme
get_data_frame()	(esmval-	method), 687
tool.diag_scripts.mlr.models.lasso_c	v.LassoCVM	
<i>method</i> ), 776	( 1	tool.diag_scripts.emergent_constraints),
<pre>get_data_frame()</pre>	(esmval-	643
	ars_cv.Lasso	olgetCNOfadeIntal_weights() (in module esmval-
method), 785		tool.diag_scripts.mlr), 661
<pre>get_data_frame()</pre>		get_image_format() (in module esmval-
<i>method</i> ), 793	LinearRegres	ssionModel tool.diag_scripts.ocean.diagnostic_tools), 864
get_data_frame()	(esmval-	get_image_path() (in module esmval-
tool.diag_scripts.mlr.models.linear_i	base.LinearN	Model tool.diag_scripts.ocean.diagnostic_tools),
<i>method</i> ), 714		864
get_data_frame()	(esmval-	<pre>get_info() (esmvaltool.diag_scripts.shared.Datasets</pre>
tool.diag_scripts.mlr.models.MLRM	odel	method), 618
<i>method</i> ), 698		<pre>get_info_list() (esmval-</pre>
get_data_frame()	(esmval-	tool.diag_scripts.shared.Datasets method),
tool.diag_scripts.mlr.models.rfr.RFR	RModel	619
<i>method</i> ), 802		<pre>get_input_data() (in module esmval-</pre>
get_data_frame()	(esmval-	tool.diag_scripts.emergent_constraints),
tool.diag_scripts.mlr.models.ridge.R	idgeModel	643
<i>method</i> ), 810	-	<pre>get_input_data() (in module esmval-</pre>
<pre>get_data_frame()</pre>	(esmval-	tool.diag_scripts.mlr), 661
tool.diag_scripts.mlr.models.ridge_c method), 818	v.RidgeCVM	Magket_input_files() (in module esmval- tool.diag_scripts.emergent_constraints),
get_data_frame()	(esmval-	644
-		
tool.diag_scripts.mlr.models.svr.SVR method), 827	inouei	<pre>get_input_files() (in module esmval- tool.diag_scripts.ocean.diagnostic_tools),</pre>
	(esmval-	865
get_data_list()		
tool.diag_scripts.shared.Datasets 617	method),	<pre>get_landsea_fraction_weights() (in module esm- valtool.diag_scripts.mlr), 662</pre>
get_dataset_info()	(esmval-	<pre>get_mean_cube() (in module esmval-</pre>

tool.diag_scripts.shared.iris_helpers), 629	aet pla	ot name()	(esmval-
		tool.diag_scripts.monitor.monitor_	X
tool.diag_scripts.mlr.custom_sklearn.Advan			
<i>method</i> ), 667	-	pt_path()	(esmval-
<pre>get_metadata_routing() (esm</pre>			
tool.diag_scripts.mlr.custom_sklearn.Advan	cedRFE		_
method), 674	get_po		esmval-
<pre>get_metadata_routing() (esm</pre>	val-	tool.diag_scripts.ocean.diagnostic	_seaice),
tool.diag_scripts.mlr.custom_sklearn.Advan	cedRFECV	860	
<i>method</i> ), 679		ovenance_record()	(esmval-
get_metadata_routing() (esm		tool.diag_scripts.monitor.monitor_	base.MonitorBase
tool.diag_scripts.mlr.custom_sklearn.Advan	•		
method), 683		ovenance_record() (in modu	
<pre>get_metadata_routing() (esm</pre>		tool.diag_scripts.emergent_constru	
tool.diag_scripts.mlr.custom_sklearn.Featur	eSelec <b>ginn/ird</b>		
method), 687	, .	tool.diag_scripts.mlr.custom_sklea	
	val- get_sea		esmval-
tool.diag_scripts.mlr.models.gpr_sklearn.Ad method), 737	ivanceaGaussi	a <b>nochoaus<u>g K</u>ugmpisco</b> cean.aiagnostic <sub>.</sub> 860	_seaice),
<pre>get_new_path() (in module esm</pre>	val- get_squ	<pre>uared_error_cube() (in modu tool.diag_scripts.mlr), 663</pre>	ıle esmval-
· · ·	<i>val-</i> get_su		(esmval-
tool.diag_scripts.ocean.diagnostic_tools),	fan gee_ba	tool.diag_scripts.mlr.custom_sklea	
865		method), 674	
get_params() (esm	<i>val-</i> get_su		(esmval-
tool.diag_scripts.mlr.custom_sklearn.Advan			rn.AdvancedRFECV
	1		
<i>method</i> ), 668		<i>method</i> ), 679	
get_params() (esm	val- get_su	pport()	(esmval-
		oport()	
<pre>get_params() (esm</pre>	<i>cedRFE</i> val- get_tir	pport() tool.diag_scripts.mlr.custom_sklea method), 688 me_string() (in module	rn.FeatureSelectionTransforme esmval-
get_params() (esm tool.diag_scripts.mlr.custom_sklearn.Advan method), 674	<i>cedRFE</i> val- get_tir	pport() tool.diag_scripts.mlr.custom_sklea method), 688 me_string() (in module	rn.FeatureSelectionTransforme esmval-
<pre>get_params() (esm tool.diag_scripts.mlr.custom_sklearn.Advan method), 674 get_params() (esm tool.diag_scripts.mlr.custom_sklearn.Advan method), 679</pre>	cedRFE val- get_tir cedRFECV	<pre>pport() tool.diag_scripts.mlr.custom_sklea method), 688 me_string() (in module tool.diag_scripts.ocean.diagnostic</pre>	rn.FeatureSelectionTransforme esmval- _seaice),
<pre>get_params() (esm tool.diag_scripts.mlr.custom_sklearn.Advan method), 674 get_params() (esm tool.diag_scripts.mlr.custom_sklearn.Advan method), 679</pre>	<i>cedRFE</i> val- get_tin <i>cedRFECV</i> val- get_tin	<pre>pport()   tool.diag_scripts.mlr.custom_sklea   method), 688 me_string() (in module   tool.diag_scripts.ocean.diagnostic   860 me_weights() (in module</pre>	rn.FeatureSelectionTransforme esmval- _seaice),
<pre>get_params() (esm</pre>	<i>cedRFE</i> val- get_tin <i>cedRFECV</i> val- get_tin	<pre>poport()   tool.diag_scripts.mlr.custom_sklea   method), 688 me_string() (in module   tool.diag_scripts.ocean.diagnostic   860 me_weights() (in module edificulgdiRggsesipts.mlr), 663 array()</pre>	rn.FeatureSelectionTransforme esmval- _seaice), esmval- (esmval-
get_params()(esmtool.diag_scripts.mlr.custom_sklearn.Advanmethod), 674get_params()(esmtool.diag_scripts.mlr.custom_sklearn.Advanmethod), 679get_params()(esmtool.diag_scripts.mlr.custom_sklearn.Advanmethod), 683get_params()(esm	cedRFE val- get_tin cedRFECV val- get_tin cedTransforme get_x_a val-	<pre>poport() tool.diag_scripts.mlr.custom_sklea method), 688 me_string() (in module tool.diag_scripts.ocean.diagnostic, 860 me_weights() (in module edifinigdiRggsesipts.mlr), 663 array() tool.diag_scripts.mlr.models.gbr_b</pre>	rn.FeatureSelectionTransforme esmval- _seaice), esmval- (esmval-
<pre>get_params() (esm</pre>	cedRFE val- get_tin cedRFECV val- get_tin cedTransforme get_x_a val- reSelectionTran	<pre>poport() tool.diag_scripts.mlr.custom_sklea method), 688 me_string() (in module tool.diag_scripts.ocean.diagnostic 860 me_weights() (in module editorgdiRggsesipts.mlr), 663 array() tool.diag_scripts.mlr.models.gbr_b asfnethed), 706</pre>	rn.FeatureSelectionTransforme esmval- _seaice), esmval- (esmval- pase.GBRModel
get_params()(esmtool.diag_scripts.mlr.custom_sklearn.Advanmethod), 674get_params()(esmtool.diag_scripts.mlr.custom_sklearn.Advanmethod), 679get_params()(esmtool.diag_scripts.mlr.custom_sklearn.Advanmethod), 683get_params()(esmtool.diag_scripts.mlr.custom_sklearn.Featurmethod), 683get_params()(esmtool.diag_scripts.mlr.custom_sklearn.Featurmethod), 687	cedRFE val- get_tin cedRFECV val- get_tin cedTransforme get_x_a val- reSelectionTran get_x_a	<pre>poport()   tool.diag_scripts.mlr.custom_sklea   method), 688 me_string() (in module   tool.diag_scripts.ocean.diagnostic   860 me_weights() (in module editodgdiRggsesipts.mlr), 663 array()   tool.diag_scripts.mlr.models.gbr_b isfoethed), 706 array()</pre>	rn.FeatureSelectionTransforme esmval- _seaice), esmval- (esmval- pase.GBRModel (esmval-
<pre>get_params() (esm</pre>	cedRFE val- get_tin cedRFECV val- get_tin cedTransforme get_x_a val- reSelectionTran get_x_a val-	<pre>poport() tool.diag_scripts.mlr.custom_sklea method), 688 me_string() (in module tool.diag_scripts.ocean.diagnostic 860 me_weights() (in module editool_diag_scripts.mlr), 663 array() tool.diag_scripts.mlr.models.gbr_b array() tool.diag_scripts.mlr.models.gbr_s</pre>	rn.FeatureSelectionTransforme esmval- _seaice), esmval- (esmval- pase.GBRModel (esmval-
<pre>get_params() (esm</pre>	cedRFE val- get_tin cedRFECV val- get_tin cedTransforme get_x_a val- reSelectionTran get_x_a val- lvancedGaussi	<pre>poport() tool.diag_scripts.mlr.custom_sklea method), 688 me_string() (in module tool.diag_scripts.ocean.diagnostic, 860 me_weights() (in module edituokdiRggsesipts.mlr), 663 array() tool.diag_scripts.mlr.models.gbr_b asfnethed), 706 array() tool.diag_scripts.mlr.models.gbr_s ianRethods,Regressor</pre>	rn.FeatureSelectionTransforme esmval- _seaice), esmval- (esmval- pase.GBRModel (esmval- klearn.SklearnGBRModel
<pre>get_params() (esm</pre>	cedRFE val- get_tin cedRFECV val- get_tin cedTransforma get_x_a val- reSelectionTran get_x_a val- lvancedGaussi get_x_a	pport() tool.diag_scripts.mlr.custom_sklea method), 688 me_string() (in module tool.diag_scripts.ocean.diagnostic 860 me_weights() (in module edifungdiRggsesipts.mlr), 663 array() tool.diag_scripts.mlr.models.gbr_b isfnethed), 706 array() tool.diag_scripts.mlr.models.gbr_s ianRthodysRegressor array()	rn.FeatureSelectionTransforme esmval- _seaice), esmval- (esmval- base.GBRModel (esmval- klearn.SklearnGBRModel (esmval-
<pre>get_params() (esm</pre>	cedRFE val- get_tin cedRFECV val- get_tin cedTransforma get_x_a val- reSelectionTran get_x_a val- lvancedGaussi get_x_a	<pre>poport() tool.diag_scripts.mlr.custom_sklea method), 688 me_string() (in module tool.diag_scripts.ocean.diagnostic, 860 me_weights() (in module edituokdiRggsesipts.mlr), 663 array() tool.diag_scripts.mlr.models.gbr_b asfnethed), 706 array() tool.diag_scripts.mlr.models.gbr_s ianRethods,Regressor</pre>	rn.FeatureSelectionTransforme esmval- _seaice), esmval- (esmval- base.GBRModel (esmval- klearn.SklearnGBRModel (esmval-
<pre>get_params() (esm</pre>	cedRFE val- get_tin cedRFECV val- get_tin cedTransforme get_x_a val- get_x_a val- lvancedGaussi get_x_a sets	poport() tool.diag_scripts.mlr.custom_sklea method), 688 me_string() (in module tool.diag_scripts.ocean.diagnostic 860 me_weights() (in module editodydiRggsesipts.mlr), 663 array() tool.diag_scripts.mlr.models.gbr_b isfnethed), 706 array() tool.diag_scripts.mlr.models.gbr_s anRthody,Regressor array() tool.diag_scripts.mlr.models.gbr_s ianRthody,Regressor array() tool.diag_scripts.mlr.models.gbr_s array() tool.diag_scripts.mlr.models.gbr_s method), 731 array()	rn.FeatureSelectionTransforme esmval- _seaice), esmval- (esmval- base.GBRModel (esmval- klearn.SklearnGBRModel (esmval- gboost.XGBoostGBRModel (esmval-
<pre>get_params() (esm</pre>	cedRFE val- get_tin cedRFECV val- get_tin cedTransforme get_x_a val- get_x_a val- lvancedGaussi get_x_a sets val- get_x_a	poport() tool.diag_scripts.mlr.custom_sklea method), 688 me_string() (in module tool.diag_scripts.ocean.diagnostic 860 me_weights() (in module editorgdiRggsesipts.mlr), 663 array() tool.diag_scripts.mlr.models.gbr_s isfnethod), 706 array() tool.diag_scripts.mlr.models.gbr_s ianRethod), Regressor array() tool.diag_scripts.mlr.models.gbr_s ianRethod), 731	rn.FeatureSelectionTransforme esmval- _seaice), esmval- (esmval- base.GBRModel (esmval- klearn.SklearnGBRModel (esmval- gboost.XGBoostGBRModel (esmval-
<pre>get_params() (esm</pre>	cedRFE val- get_tin cedRFECV val- get_tin cedTransforme get_x_a val- get_x_a val- lvancedGaussi get_x_a sets val- get_x_a	pport() tool.diag_scripts.mlr.custom_sklea method), 688 me_string() (in module tool.diag_scripts.ocean.diagnostic, 860 me_weights() (in module edifungdiRggsesipts.mlr), 663 array() tool.diag_scripts.mlr.models.gbr_b isfnethed), 706 array() tool.diag_scripts.mlr.models.gbr_s ianRethody,Regressor array() tool.diag_scripts.mlr.models.gbr_s method), 731 array() tool.diag_scripts.mlr.models.gbr_s method), 744	rn.FeatureSelectionTransforme esmval- _seaice), esmval- (esmval- base.GBRModel (esmval- klearn.SklearnGBRModel (esmval- gboost.XGBoostGBRModel (esmval-
<pre>get_params() (esm</pre>	cedRFE val- get_tin cedRFECV val- get_tin cedTransforme get_x_a val- get_x_a val- dvancedGaussi get_x_a sets val- get_x_a od),	pport() tool.diag_scripts.mlr.custom_sklea method), 688 me_string() (in module tool.diag_scripts.ocean.diagnostic, 860 me_weights() (in module edifungdiRggsesipts.mlr), 663 array() tool.diag_scripts.mlr.models.gbr_b isfnethed), 706 array() tool.diag_scripts.mlr.models.gbr_s ianRethody,Regressor array() tool.diag_scripts.mlr.models.gbr_s method), 731 array() tool.diag_scripts.mlr.models.gbr_s method), 744	rn.FeatureSelectionTransforme esmval- _seaice), esmval- (esmval- base.GBRModel (esmval- klearn.SklearnGBRModel (esmval- gboost.XGBoostGBRModel (esmval- klearn.SklearnGPRModel (esmval-
<pre>get_params() (esm</pre>	cedRFE val- get_tin cedRFECV val- get_tin cedTransforme get_x_a val- reSelectionTran get_x_a val- lvancedGaussi get_x_a sets val- get_x_a val- dvancedGaussi get_x_a val- yal-	poport() tool.diag_scripts.mlr.custom_sklea method), 688 me_string() (in module tool.diag_scripts.ocean.diagnostic 860 me_weights() (in module editorgdiRggseripts.mlr), 663 array() tool.diag_scripts.mlr.models.gbr_b isfnethed), 706 array() tool.diag_scripts.mlr.models.gbr_s anRethod), 706 array() tool.diag_scripts.mlr.models.gbr_s method), 731 array() tool.diag_scripts.mlr.models.gpr_s method), 744 array() tool.diag_scripts.mlr.models.gpr_s method), 744 array() tool.diag_scripts.mlr.models.huben method), 752	rn.FeatureSelectionTransforme esmval- _seaice), esmval- (esmval- base.GBRModel (esmval- klearn.SklearnGBRModel (esmval- gboost.XGBoostGBRModel (esmval- klearn.SklearnGPRModel (esmval- :HuberRegressionModel
<pre>get_params() (esm</pre>	cedRFE val- get_tim cedRFECV val- get_tim cedTransforme get_x_a val- reSelectionTran get_x_a val- lvancedGaussi get_x_a val- get_x_a	poport() tool.diag_scripts.mlr.custom_sklea method), 688 me_string() (in module tool.diag_scripts.ocean.diagnostic 860 me_weights() (in module editorgdiRggsesipts.mlr), 663 array() tool.diag_scripts.mlr.models.gbr_b isfnethed), 706 array() tool.diag_scripts.mlr.models.gbr_s ianRethod), 706 array() tool.diag_scripts.mlr.models.gbr_s method), 731 array() tool.diag_scripts.mlr.models.gpr_s method), 744 array() tool.diag_scripts.mlr.models.huber method), 752 array()	rn.FeatureSelectionTransforme esmval- _seaice), esmval- (esmval- base.GBRModel (esmval- klearn.SklearnGBRModel (esmval- gboost.XGBoostGBRModel (esmval- klearn.SklearnGPRModel (esmval- :HuberRegressionModel (esmval-
<pre>get_params() (esm</pre>	cedRFE val- get_tir cedRFECV val- get_tir cedTransforme get_x_a val- get_x_a val- dvancedGaussi get_x_a sets val- get_x_a val- get_x_a val- get_x_a val- get_x_a	poport() tool.diag_scripts.mlr.custom_sklea method), 688 me_string() (in module tool.diag_scripts.ocean.diagnostic 860 me_weights() (in module editodgdiRggsesipts.mlr), 663 array() tool.diag_scripts.mlr.models.gbr_b isfnethod), 706 array() tool.diag_scripts.mlr.models.gbr_s ianRethodys,Regressor array() tool.diag_scripts.mlr.models.gbr_s method), 731 array() tool.diag_scripts.mlr.models.gpr_s method), 744 array() tool.diag_scripts.mlr.models.huben method), 752 array() tool.diag_scripts.mlr.models.huben method), 752 array() tool.diag_scripts.mlr.models.krr.K.	rn.FeatureSelectionTransforme esmval- _seaice), esmval- (esmval- base.GBRModel (esmval- klearn.SklearnGBRModel (esmval- gboost.XGBoostGBRModel (esmval- klearn.SklearnGPRModel (esmval- :HuberRegressionModel (esmval-
<pre>get_params() (esm tool.diag_scripts.mlr.custom_sklearn.Advan method), 674 get_params() (esm tool.diag_scripts.mlr.custom_sklearn.Advan method), 679 get_params() (esm tool.diag_scripts.mlr.custom_sklearn.Advan method), 683 get_params() (esm tool.diag_scripts.mlr.custom_sklearn.Featur method), 687 get_params() (esm tool.diag_scripts.mlr.models.gpr_sklearn.Advan method), 738 get_path() (esmvaltool.diag_scripts.shared.Data method), 619 get_path_list() (esm tool.diag_scripts.shared.Datasets metho 619 get_path_to_mpl_style() (in module esm tool.diag_scripts.shared.plot), 631 get_plot_filename() (in module esm tool.diag_scripts.shared.plot), 625</pre>	cedRFE val- get_tir cedRFECV val- get_tir cedTransforme get_x_a val- get_x_a val- dvancedGaussi get_x_a sets val- get_x_a val- get_x_a val- get_x_a val- get_x_a	poport() tool.diag_scripts.mlr.custom_sklea method), 688 me_string() (in module tool.diag_scripts.ocean.diagnostic 860 me_weights() (in module editodgdiRggsesipts.mlr), 663 array() tool.diag_scripts.mlr.models.gbr_b isfnethoed), 706 array() tool.diag_scripts.mlr.models.gbr_s ianPethoed), Regressor array() tool.diag_scripts.mlr.models.gbr_s method), 731 array() tool.diag_scripts.mlr.models.gpr_s method), 744 array() tool.diag_scripts.mlr.models.huber method), 752 array() tool.diag_scripts.mlr.models.huber method), 752 array() tool.diag_scripts.mlr.models.krr.Ki method), 760	rn.FeatureSelectionTransforme esmval- _seaice), esmval- (esmval- base.GBRModel (esmval- klearn.SklearnGBRModel (esmval- gboost.XGBoostGBRModel (esmval- klearn.SklearnGPRModel (esmval- :HuberRegressionModel (esmval-

tool.diag_scripts.mlr.models.lasso.La	ssoModel		method), 77	7			
<i>method</i> ), 768		get_y_a	array()			(esmval-	
get_x_array()	(esmval-			ripts.ml	r.models.lass	so_lars_cv.LassoLarsCVMo	del
tool.diag_scripts.mlr.models.lasso_cv	.LassoCVM	lodel	method), 785	5			
<i>method</i> ), 776		get_y_a	array()			(esmval-	
<pre>get_x_array()</pre>	(esmval-		tool.diag_sc.	ripts.ml	r.models.line	ar.LinearRegressionModel	
tool.diag_scripts.mlr.models.lasso_la	ers_cv.Lasso	LarsCVM	onthethod), 794	4		-	
method), 785		get_y_a				(esmval-	
<pre>get_x_array()</pre>	(esmval-	•		ripts.ml	r.models.line	ear_base.LinearModel	
tool.diag_scripts.mlr.models.linear.Li	inearRegres	sionMode					
method), 793	0	get_y_a				(esmval-	
<pre>get_x_array()</pre>	(esmval-	5 )	tool.diag_sc	ripts.ml	r.models.ML		
tool.diag_scripts.mlr.models.linear_b		Model					
method), 714	use.Emeuri	get_y_a		0		(esmval-	
get_x_array()	(esmval-	gcc_y_c	tool.diag_sc.	rints ml	rmodels rfr		
tool.diag_scripts.mlr.models.MLRMo			method), 802		oucis.iji.i	in Innouci	
method), 698	uei	aot v		2		(esmval-	
	(asmual	get_y_a		winte ml	n madala nida		
get_x_array()	(esmval-				r.models.ridg	ge.RidgeModel	
tool.diag_scripts.mlr.models.rfr.RFR	model		method), 810	0		(	
method), 802	( 1	get_y_a	-	•		(esmval-	
<pre>get_x_array()</pre>	(esmval-		-	-	r.models.ridg	ge_cv.RidgeCVModel	
tool.diag_scripts.mlr.models.ridge.Rid	dgeModel		method), 819	9		<i>,</i>	
method), 810		get_y_a	-			(esmval-	
<pre>get_x_array()</pre>	(esmval-		tool.diag_sc		r.models.svr.	SVRModel	
tool.diag_scripts.mlr.models.ridge_cv	.RidgeCVM		method), 827				
<i>method</i> ), 818		get_yea		(in	module	esmval-	
get_x_array()	(esmval-		tool.diag_sc	ripts.oc	ean.diagnost	ic_seaice),	
tool.diag_scripts.mlr.models.svr.SVR	Model		860				
<i>method</i> ), 827		global_	_contourf()	(ir	1 modul	le esmval-	
<pre>get_xy_data_without_nans() (in module</pre>	e esmval-		tool.diag_sc	ripts.sh	ared.plot), 63	31	
tool.diag_scripts.emergent_constrain	ts), 644	global_	_pcolormesh	l()	(in modu	ıle esmval-	
get_y_array()	(esmval-		tool.diag_sc	ripts.she	ared.plot), 63	31	
tool.diag_scripts.mlr.models.gbr_bas	e.GBRMode	<i>el</i> grid_se	earch_cv()			(esmval-	
method), 706			tool.diag_sc	ripts.ml	r.models.gbr	_base.GBRModel	
get_y_array()	(esmval-		method), 70	7	-		
tool.diag_scripts.mlr.models.gbr_skle	earn.Sklearr	ıGBRMse	lahrch_cv()			(esmval-	
method), 723		-		ripts.ml	r.models.gbr	_sklearn.SklearnGBRModel	l
get_y_array()	(esmval-		method), 723	-	0		
tool.diag_scripts.mlr.models.gbr_xgb	oost.XGBoo	os <b>aGBRM</b> a				(esmval-	
<i>method</i> ), 731		5 –		ripts.ml	r.models.gbr	_xgboost.XGBoostGBRMod	lel
get_y_array()	(esmval-		method), 732	·			
tool.diag_scripts.mlr.models.gpr_skle		∩G₽RMaa	<i>,,</i>	-		(esmval-	
method), 744	an montean i	/91 101100		rints ml	rmodels onr	_sklearn.SklearnGPRModel	1
get_y_array()	(esmval-		method), 74	-			/
tool.diag_scripts.mlr.models.huber.H		cienn Marka	<i>,,</i>	5		(esmval-	
method), 752	ubernegres.	sigund <u>a</u> a		rints ml	rmodels hub	er.HuberRegressionModel	
get_y_array()	(esmval-		method), 753	-		er.muderKegressionmoder	
		anid a		5		(esmval-	
tool.diag_scripts.mlr.models.krr.KRR	model	gr1u_se	earch_cv()				
method), 761	<i>(</i> 1		tool.diag_sc	·	r.models.krr.	KKKMOdel	
<pre>get_y_array()</pre>	(esmval-		method), 76	1		( 1	
tool.diag_scripts.mlr.models.lasso.La	lssoModel	grıd_se	earch_cv()			(esmval-	
method), 768							
	/ 1		tool.diag_sc	-	r.models.lass	so.LassoModel	
<pre>get_y_array()</pre>	(esmval-		method), 769	-	r.models.lass	so.LassoModel (esmval-	

tool.diag_scripts.mlr.models.lasso_cv. method), 777	LassoCVM		tool.diag_scripts property), 794	.mlr.models.linear.Li	nearRegressionModel
	(esmval-		ttributes		(esmval-
tool.diag_scripts.mlr.models.lasso_lar				mlrmodals linear b	•
method), 786	s_cv.Lusso				use.Lineumouei
	( annual		property), 715		( again al
			ttributes		(esmval-
tool.diag_scripts.mlr.models.linear.Lin	iearKegres			s.mir.moaeis.MLRMoo	ael
method), 794	/ <b>1</b>		property), 699		,
-			ttributes		(esmval-
tool.diag_scripts.mlr.models.linear_ba	ise.LinearN		° .	.mlr.models.rfr.RFRM	Aodel
<i>method</i> ), 715			property), 803		
-	(esmval-		ttributes		(esmval-
tool.diag_scripts.mlr.models.MLRMod	lel		tool.diag_scripts	.mlr.models.ridge.Ric	lgeModel
method), 699			property), 811		
grid_search_cv()	(esmval-	group_a	ttributes		(esmval-
tool.diag_scripts.mlr.models.rfr.RFRM	lodel		tool.diag_scripts	.mlr.models.ridge_cv.	RidgeCVModel
<i>method</i> ), 803			property), 819		
grid_search_cv()	(esmval-	group_a	ttributes		(esmval-
tool.diag_scripts.mlr.models.ridge.Rid	geModel		tool.diag_scripts	.mlr.models.svr.SVRM	Model
method), 811			property), 828		
	(esmval-		etadata()	(in module	esmval-
tool.diag_scripts.mlr.models.ridge_cv.			tool.diag_scripts		
<i>method</i> ), 819	0.0			<pre>ime() (in module</pre>	esmval-
grid_search_cv()	(esmval-	-		.ocean.diagnostic_to	
tool.diag_scripts.mlr.models.svr.SVRM			865	io contrata gito site_io	,
method), 828	louei		005		
	(esmval-	Н			
tool.diag_scripts.mlr.models.gbr_base	<b>`</b>		araccionModal	(class in	esmval-
property), 707	.ODM/////		-		
	(esmval-		iooi.aiag_scripis	.mlr.models.huber), 7	/49
tool.diag_scripts.mlr.models.gbr_sklea		topmad	al		
	im.skieum		el		
property), 723					
	(	ignore_	warnings()	(in module	esmval-
group_attributes	(esmval-	-	tool.diag_scripts	.mlr), 663	
<pre>group_attributes</pre>		-	tool.diag_scripts	•	
<pre>group_attributes</pre>	ost.XGBoo	ogeneration of the second s	tool.diag_scripts del (esmvaltoo method), 621	s.mlr), 663 ol.diag_scripts.shared	l.Variable
<pre>group_attributes</pre>	ost.XGBoo (esmval-	Sinterso	tool.diag_scripts del (esmvaltoo method), 621	s.mlr), 663 ol.diag_scripts.shared	l.Variable
<pre>group_attributes</pre>	ost.XGBoo (esmval-	Sinterso	tool.diag_scripts del (esmvaltoo method), 621	s.mlr), 663 ol.diag_scripts.shared	l.Variable
<pre>group_attributes</pre>	oost.XGBoo (esmval- urn.Sklearn	interse	tool.diag_scripts del (esmvaltoo method), 621	s.mlr), 663 ol.diag_scripts.shared	l.Variable
<pre>group_attributes</pre>	oost.XGBoo (esmval- urn.Sklearn (esmval-	interse GPRMode	tool.diag_scripts del (esmvaltoo method), 621 ct_dataset_coo valtool.diag_scru _transform() tool diag_scripts	s.mlr), 663 ol.diag_scripts.shared	l.Variable dule esm- rs), 629 (esmval-
<pre>group_attributes             tool.diag_scripts.mlr.models.gbr_xgbo             property), 732 group_attributes             tool.diag_scripts.mlr.models.gpr_skled             property), 745</pre>	oost.XGBoo (esmval- urn.Sklearn (esmval-	interse GPRMode	tool.diag_scripts del (esmvaltoo method), 621 ct_dataset_coo valtool.diag_scru _transform() tool diag_scripts	s.mlr), 663 ol.diag_scripts.shared ordinates() (in mo ipts.shared.iris_helpe	l.Variable dule esm- rs), 629 (esmval-
<pre>group_attributes</pre>	oost.XGBoo (esmval- urn.Sklearn (esmval-	interse GPRModa inverse sionModel	tool.diag_scripts del (esmvaltoo method), 621 ct_dataset_coo valtool.diag_scri _transform() tool.diag_scripts method), 668	s.mlr), 663 ol.diag_scripts.shared ordinates() (in mo ipts.shared.iris_helpe	l.Variable dule esm- rs), 629 (esmval- AdvancedPipeline
<pre>group_attributes</pre>	oost.XGBoo (esmval- urn.Sklearn (esmval-	interse GPRModa inverse sionModel	tool.diag_scripts del (esmvaltoo method), 621 ct_dataset_coo valtool.diag_scripts method), 668 _transform()	.mlr), 663 ol.diag_scripts.shared ordinates() (in mo ipts.shared.iris_helpe c.mlr.custom_sklearn	l.Variable dule esm- rs), 629 (esmval- AdvancedPipeline (esmval-
<pre>group_attributes</pre>	ost.XGBoo (esmval- urn.Sklearn (esmval- berRegress (esmval-	interse GPRMode inverse sionModel inverse	tool.diag_scripts del (esmvaltoo method), 621 ct_dataset_coo evaltool.diag_scripts method), 668 _transform() tool.diag_scripts	s.mlr), 663 ol.diag_scripts.shared ordinates() (in mo ipts.shared.iris_helpe	l.Variable dule esm- rs), 629 (esmval- AdvancedPipeline (esmval-
<pre>group_attributes</pre>	ost.XGBoo (esmval- urn.Sklearn (esmval- berRegress (esmval-	interse GPRMode inverse sionModel inverse	tool.diag_scripts del (esmvaltoo method), 621 ct_dataset_cou evaltool.diag_scripts method), 668 _transform() tool.diag_scripts method), 674	.mlr), 663 ol.diag_scripts.shared ordinates() (in mo ipts.shared.iris_helpe c.mlr.custom_sklearn	l.Variable dule esm- rs), 629 (esmval- AdvancedPipeline (esmval- AdvancedRFE
<pre>group_attributes</pre>	ost.XGBoo (esmval- urn.Sklearn (esmval- berRegress (esmval-	interse GPRMode inverse sionModel inverse	tool.diag_scripts del (esmvaltoo method), 621 ct_dataset_cou evaltool.diag_scripts method), 668 _transform() tool.diag_scripts method), 674 _transform()	.mlr), 663 ol.diag_scripts.shared ordinates() (in mo ipts.shared.iris_helpe c.mlr.custom_sklearn	l.Variable dule esm- rs), 629 (esmval- AdvancedPipeline (esmval- AdvancedRFE (esmval-
<pre>group_attributes</pre>	ost.XGBoo (esmval- urn.Sklearn (esmval- berRegress (esmval- lodel (esmval-	interse GPRMode inverse sionModel inverse	tool.diag_scripts del (esmvaltoo method), 621 ct_dataset_coo valtool.diag_scripts method), 668 _transform() tool.diag_scripts method), 674 _transform() tool.diag_scripts method), 674	.mlr), 663 ol.diag_scripts.shared ordinates() (in mo ipts.shared.iris_helpe c.mlr.custom_sklearn	l.Variable dule esm- rs), 629 (esmval- AdvancedPipeline (esmval- AdvancedRFE (esmval-
group_attributes tool.diag_scripts.mlr.models.gbr_xgbo property), 732 group_attributes tool.diag_scripts.mlr.models.gpr_skled property), 745 group_attributes tool.diag_scripts.mlr.models.huber.Hu property), 753 group_attributes tool.diag_scripts.mlr.models.krr.KRRM property), 761	ost.XGBoo (esmval- urn.Sklearn (esmval- berRegress (esmval- lodel (esmval-	interse GPRMode inverse sionModel inverse	tool.diag_scripts del (esmvaltoo method), 621 ct_dataset_coo valtool.diag_scripts method), 668 _transform() tool.diag_scripts method), 674 _transform() tool.diag_scripts method), 679	.mlr), 663 ol.diag_scripts.shared ordinates() (in mo ipts.shared.iris_helpe c.mlr.custom_sklearn	l.Variable dule esm- rs), 629 (esmval- AdvancedPipeline (esmval- AdvancedRFE (esmval- AdvancedRFECV
<pre>group_attributes</pre>	ost.XGBoo (esmval- urn.Sklearn (esmval- berRegress (esmval- lodel (esmval-	interse GPRMode inverse sionModel inverse	tool.diag_scripts del (esmvaltoo method), 621 ct_dataset_coo valtool.diag_scripts method), 668 _transform() tool.diag_scripts method), 674 _transform() tool.diag_scripts method), 679 _transform()	.mlr), 663 ol.diag_scripts.shared ordinates() (in mo ipts.shared.iris_helpe s.mlr.custom_sklearn s.mlr.custom_sklearn	l.Variable dule esm- rs), 629 (esmval- AdvancedPipeline (esmval- AdvancedRFE (esmval- AdvancedRFECV (esmval-
<pre>group_attributes</pre>	ost.XGBoo (esmval- arn.Sklearn (esmval- berRegress (esmval- 10del (esmval- soModel (esmval-	interse GPRMode inverse sionModel inverse inverse	tool.diag_scripts del (esmvaltoo method), 621 ct_dataset_coo evaltool.diag_scripts method), 668 _transform() tool.diag_scripts method), 674 _transform() tool.diag_scripts method), 679 _transform() tool.diag_scripts method), 679 _transform()	.mlr), 663 ol.diag_scripts.shared ordinates() (in mo ipts.shared.iris_helpe s.mlr.custom_sklearn s.mlr.custom_sklearn	l.Variable dule esm- rs), 629 (esmval- AdvancedPipeline (esmval- AdvancedRFE (esmval- AdvancedRFECV
<pre>group_attributes</pre>	ost.XGBoo (esmval- arn.Sklearn (esmval- berRegress (esmval- 10del (esmval- soModel (esmval-	interse GPRMode inverse sionModel inverse inverse	tool.diag_scripts del (esmvaltoo method), 621 ct_dataset_cou evaltool.diag_scripts method), 668 _transform() tool.diag_scripts method), 674 _transform() tool.diag_scripts method), 679 _transform() tool.diag_scripts method), 679 _transform() tool.diag_scripts method), 688	.mlr), 663 ol.diag_scripts.shared ordinates() (in mo ipts.shared.iris_helpe .mlr.custom_sklearn .mlr.custom_sklearn .mlr.custom_sklearn	l.Variable dule esm- rs), 629 (esmval- AdvancedPipeline (esmval- AdvancedRFE (esmval- AdvancedRFECV (esmval- FeatureSelectionTransforme
<pre>group_attributes</pre>	ost.XGBoo (esmval- arn.Sklearn (esmval- berRegress (esmval- 10del (esmval- soModel (esmval-	interse GPRMode inverse sionModel inverse inverse	tool.diag_scripts del (esmvaltoo method), 621 ct_dataset_cou evaltool.diag_scripts method), 668 _transform() tool.diag_scripts method), 674 _transform() tool.diag_scripts method), 679 _transform() tool.diag_scripts method), 679 _transform() tool.diag_scripts method), 688 ct() (esmvaltool	.mlr), 663 ol.diag_scripts.shared ordinates() (in mo ipts.shared.iris_helpe s.mlr.custom_sklearn s.mlr.custom_sklearn	l.Variable dule esm- rs), 629 (esmval- AdvancedPipeline (esmval- AdvancedRFE (esmval- AdvancedRFECV (esmval- FeatureSelectionTransforme
<pre>group_attributes</pre>	ost.XGBoo (esmval- urn.Sklearn (esmval- berRegress (esmval- lodel (esmval- soModel (esmval- LassoCVM (esmval-	interse GGPRModel inverse sionModel inverse inverse inverse dodel iris_di	tool.diag_scripts del (esmvaltoo method), 621 ct_dataset_coo valtool.diag_scripts method), 668 _transform() tool.diag_scripts method), 674 _transform() tool.diag_scripts method), 679 _transform() tool.diag_scripts method), 679 _transform() tool.diag_scripts method), 688 ct() (esmvaltool method), 623	.mlr), 663 ol.diag_scripts.shared ordinates() (in mo ipts.shared.iris_helpe s.mlr.custom_sklearn s.mlr.custom_sklearn s.mlr.custom_sklearn s.mlr.custom_sklearn	l.Variable dule esm- rs), 629 (esmval- AdvancedPipeline (esmval- AdvancedRFE (esmval- AdvancedRFECV (esmval- FeatureSelectionTransforme Variables
<pre>group_attributes</pre>	ost.XGBoo (esmval- urn.Sklearn (esmval- berRegress (esmval- lodel (esmval- soModel (esmval- LassoCVM (esmval-	interse GGPRModel inverse sionModel inverse inverse inverse dodel iris_di	tool.diag_scripts del (esmvaltoo method), 621 ct_dataset_coo evaltool.diag_scripts method), 668 _transform() tool.diag_scripts method), 668 _transform() tool.diag_scripts method), 674 _transform() tool.diag_scripts method), 679 _transform() tool.diag_scripts method), 679 _transform() tool.diag_scripts method), 679 _transform() tool.diag_scripts method), 688 ct() (esmvaltool method), 623 offect_constra:	.mlr), 663 ol.diag_scripts.shared ordinates() (in mo ipts.shared.iris_helpe s.mlr.custom_sklearn s.mlr.custom_sklearn s.mlr.custom_sklearn s.mlr.custom_sklearn	l.Variable dule esm- rs), 629 (esmval- AdvancedPipeline (esmval- AdvancedRFE (esmval- AdvancedRFECV (esmval- FeatureSelectionTransforme Variables esmval-

К		property), 761
KRRModel (class in esmval-	label_	
tool.diag_scripts.mlr.models.krr), 757		tool.diag_scripts.mlr.models.lasso.LassoModel
toot.uug_seripis.nutinoueis.wr/, 191		property), 769
L	label_	
<pre>label (esmvaltool.diag_scripts.mlr.models.gbr_base.GBF property), 707</pre>	RModel	tool.diag_scripts.mlr.models.lasso_cv.LassoCVModel property), 777
label (esmvaltool.diag_scripts.mlr.models.gbr_sklearn.S	ulabel	(esmval-
property), 723		iooi.uug_scripis.mir.modeis.iusso_iurs_cv.LussoLurscv.Modei
label (esmvaltool.diag_scripts.mlr.models.gbr_xgboost.X	GBoostGl	RRNPRATY), 786
<pre>label(esmvaltool.diag_scripts.mlr.models.gpr_sklearn.S property), 745</pre>		RModel property), 794
label (esmvaltool.diag_scripts.mlr.models.huber.HuberR	egression!	units (esmval-
property), 753	0	ioonanag_senipisinininioueisininean_buselBineaninouei
label (esmvaltool.diag_scripts.mlr.models.krr.KRRMode	l	property), 715
property), 761	label_	
label (esmvaltool.diag_scripts.mlr.models.lasso.LassoMe	odel	tool.diag_scripts.mlr.models.MLRModel
property) 769		property), 699
label (esmvaltool.diag_scripts.mlr.models.lasso_cv.Lass	oCVM8del	units (esmval-
property) 777		ioonalas_seripis.inininoaeis.iji.iti Tanoaei
label (esmvaltool.diag_scripts.mlr.models.lasso_lars_cv. property), 786	LassoLars	CV(Deerty), 803
property), 786	Taper_	units (esmval-
label (esmvaltool.diag_scripts.mlr.models.linear.Lineark property), 794		property), or
label (esmvaltool.diag_scripts.mlr.models.linear_base.L	inearMode	units (esmval-
property), 715		loonalag_seripis.inininouels.ruge_erintugee rinouel
label (esmvaltool.diag_scripts.mlr.models.MLRModel		property), 819
property), 699	label_	× ·
<pre>label (esmvaltool.diag_scripts.mlr.models.rfr.RFRModel property) 803</pre>		tool.diag_scripts.mlr.models.svr.SVRModel property), 828
label (esmvaltool.diag_scripts.mlr.models.ridge.RidgeMo	del LassoC	VModel (class in esmval-
nroperty 811		1001.aua5_501.p15.int1.int0.act5.ia550_07), 775
label (esmvaltool.diag_scripts.mlr.models.ridge_cv.Ridge	eCVM88el	arsCVModel (class in esmval-
<i>property</i> ), 819		
label (esmvaltool.diag_scripts.mlr.models.svr.SVRModel		781
property), 828	LassoM	
lahel units (esmual-	- •	tool.diag_scripts.mlr.models.lasso), 765
tool.diag_scripts.mlr.models.gbr_base.GBRMod	<i>lel</i> Linear	Model (class in esmval-
property), 707		iooi.uug_scripis.mir.moucis.incur_buse),
lahel units (esmval-		
tool.diag_scripts.mlr.models.gbr_sklearn.Sklear	nGBRMb	RegressionModel (class in esmval-
property), 723		iooi.uug_scripis.mii.moueis.uneur), 790
label_units (esmval-	1οαα_τι	hresholds() (in module esmval-
tool.diag_scripts.mlr.models.gbr_xgboost.XGBc	ostGBRM	odel.diag_scripts.ocean.diagnostic_toois),
property), 732		005
label_units (esmval-		esmvaltool.diag_scripts.shared.ProvenanceLogger
tool.diag_scripts.mlr.models.gpr_sklearn.Sklear	nGPRMod	del <sup>l</sup> enod), 621 rginal_likelihood() ( <i>esmval</i> -
property), 745	10 <u>9_</u> ma.	tool.diag_scripts.mlr.models.gpr_sklearn.AdvancedGaussianProd
label_units (esmval-		· · · · · · · · · · · · · · · · · · ·
tool.diag_scripts.mlr.models.huber.HuberRegre	ssionMode	ame (esmvaltool.diag_scripts.shared.Variable at-
property), 753	TOUR TO	tribute), 622
label_units (esmval-	long n	ame() (esmvaltool.diag_scripts.shared.Variables
tool.diag_scripts.mlr.models.krr.KRRModel	TOUR	ame() (esinvanoon.aag_seripis.snarea.variaores

method), 623

#### Μ

- main() (in module esmvaltool.diag\_scripts.ocean.diagnostic\_maps), 846
- main() (in module esmvaltool.diag\_scripts.ocean.diagnostic\_maps\_quad), 848
- main() (in module esmvaltool.diag\_scripts.ocean.diagnostic\_profiles), 852
- main() (in module esmvaltool.diag\_scripts.ocean.diagnostic\_seaice), 860
- main() (in module esmvaltool.diag\_scripts.ocean.diagnostic\_timeseries), 853
- main() (in module esmvaltool.diag\_scripts.ocean.diagnostic\_transects), 856
- make\_cube\_layer\_dict() (in module esmvaltool.diag\_scripts.ocean.diagnostic\_tools), 866
- make\_cube\_region\_dict() (in module esmvaltool.diag\_scripts.ocean.diagnostic\_transects), 856
- make\_depth\_safe() (in module esmvaltool.diag\_scripts.ocean.diagnostic\_transects), 856
- make\_map\_contour() (in module esmvaltool.diag\_scripts.ocean.diagnostic\_maps), 847
- make\_map\_extent\_plots() (in module esmvaltool.diag\_scripts.ocean.diagnostic\_seaice), 860
- make\_map\_plots() (in module esmvaltool.diag\_scripts.ocean.diagnostic\_maps), 847
- make\_map\_plots() (in module esmvaltool.diag\_scripts.ocean.diagnostic\_seaice), 861
- make\_polar\_map() (in module esmvaltool.diag\_scripts.ocean.diagnostic\_seaice), 861
- make\_profiles\_plots() (in module esmvaltool.diag\_scripts.ocean.diagnostic\_profiles), 852

- make\_scatter() (in module esmvaltool.diag scripts.ocean.diagnostic model vs obs), 851 make\_time\_series\_plots() (in module esmvaltool.diag scripts.ocean.diagnostic timeseries), 854 make transect contours() (in module esmvaltool.diag scripts.ocean.diagnostic transects), 857 make\_transects\_plots() (in module esmvaltool.diag\_scripts.ocean.diagnostic\_transects), 857 esmval- make\_ts\_plots() module (in esmval
  - tool.diag\_scripts.ocean.diagnostic\_seaice),
    861
    match\_model\_to\_key() (in module esmval-
  - tool.diag\_scripts.ocean.diagnostic\_tools), 866
  - mlr\_model\_type (esmvaltool.diag\_scripts.mlr.models.gbr\_base.GBRModel property), 707
  - mlr\_model\_type (esmvaltool.diag\_scripts.mlr.models.gbr\_sklearn.SklearnGBRModel property), 724
  - mlr\_model\_type (esmvaltool.diag\_scripts.mlr.models.gbr\_xgboost.XGBoostGBRModel property), 732
  - mlr\_model\_type (esmvaltool.diag\_scripts.mlr.models.gpr\_sklearn.SklearnGPRModel property), 745
  - mlr\_model\_type (esmvaltool.diag\_scripts.mlr.models.huber.HuberRegressionModel property), 753
  - mlr\_model\_type (esmvaltool.diag\_scripts.mlr.models.krr.KRRModel property), 761
  - mlr\_model\_type (esmvaltool.diag\_scripts.mlr.models.lasso.LassoModel property), 769
  - mlr\_model\_type (esmvaltool.diag\_scripts.mlr.models.lasso\_cv.LassoCVModel property), 777
  - mlr\_model\_type (esmvaltool.diag\_scripts.mlr.models.lasso\_lars\_cv.LassoLarsCVModel property), 786
    - .r\_model\_type (esmvaltool.diag\_scripts.mlr.models.linear.LinearRegressionModel property), 795
  - mlr\_model\_type (esmvaltool.diag\_scripts.mlr.models.linear\_base.LinearModel property), 715
  - mlr\_model\_type (esmvaltool.diag\_scripts.mlr.models.MLRModel property), 699

<pre>mlr_model_type</pre>	(esmval-	<pre>esmvaltool.diag_scripts.mlr.models.linear, 790</pre>
0— 1 V	Model	
property), 803	(	<pre>esmvaltool.diag_scripts.mlr.models.linear_base, 711</pre>
mlr_model_type	(esmval-	
tool.diag_scripts.mlr.models.ridge.R	lidgeModel	<pre>esmvaltool.diag_scripts.mlr.models.rfr,</pre>
property), 811	<i>,</i> ,	798
mlr_model_type	(esmval-	<pre>esmvaltool.diag_scripts.mlr.models.ridge,</pre>
tool.diag_scripts.mlr.models.ridge_c	cv.RidgeCVModel	
property), 819		<pre>esmvaltool.diag_scripts.mlr.models.ridge_cv,</pre>
mlr_model_type	(esmval-	815
tool.diag_scripts.mlr.models.svr.SVI	RModel	<pre>esmvaltool.diag_scripts.mlr.models.svr,</pre>
property), 828		823
MLRModel (class in esmvaltool.diag_scripts.m	ılr.models),	<pre>esmvaltool.diag_scripts.mlr.plot,651</pre>
695		<pre>esmvaltool.diag_scripts.mlr.postprocess,</pre>
<pre>modify_var()</pre>	(esmval-	653
tool.diag_scripts.shared.Variables	method),	<pre>esmvaltool.diag_scripts.mlr.preprocess,</pre>
623		655
module		<pre>esmvaltool.diag_scripts.mlr.rescale_with_emergent_cons</pre>
<pre>esmvaltool.diag_scripts.emergen</pre>	t_constraints.	
639	_ ,	<pre>esmvaltool.diag_scripts.monitor.compute_eofs,</pre>
esmvaltool.diag_scripts.emergen	t constraints.	
635		esmvaltool.diag_scripts.monitor.monitor,
esmvaltool.diag_scripts.emergen	t constraints	
636	<u></u>	esmvaltool.diag_scripts.monitor.monitor_base,
esmvaltool.diag_scripts.emergen	t constraints	
637	L_CONSTRAINTS.	
		<pre>esmvaltool.diag_scripts.monitor.multi_datasets,</pre>
esmvaltool.diag_scripts.emergen	t_constraints.	
638		<pre>esmvaltool.diag_scripts.ocean.diagnostic_maps,</pre>
esmvaltool.diag_scripts.mlr,658		846
esmvaltool.diag_scripts.mlr.cus 664	tom_sklearn,	<pre>esmvaltool.diag_scripts.ocean.diagnostic_maps_quad,</pre>
	luate residual	<pre>sesmvaltool.diag_scripts.ocean.diagnostic_model_vs_obs,</pre>
648		848
esmvaltool.diag_scripts.mlr.main	n 649	esmvaltool.diag_scripts.ocean.diagnostic_profiles,
esmvaltool.diag_scripts.mlr.mmm,		851
esmvaltool.diag_scripts.mlr.mode		esmvaltool.diag_scripts.ocean.diagnostic_seaice,
esmvaltool.diag_scripts.mlr.mod		857
703	ers.gur_base,	
,	le charableau	<pre>esmvaltool.diag_scripts.ocean.diagnostic_timeseries,</pre>
esmvaltool.diag_scripts.mlr.mode	eis.gbr_skiear	
719		<pre>esmvaltool.diag_scripts.ocean.diagnostic_tools,</pre>
esmvaltool.diag_scripts.mlr.mode	els.gbr_xgboos	
728		<pre>esmvaltool.diag_scripts.ocean.diagnostic_transects,</pre>
esmvaltool.diag_scripts.mlr.mod	els.gpr_sklear	
736		<pre>esmvaltool.diag_scripts.psyplot_diag, 867</pre>
<pre>esmvaltool.diag_scripts.mlr.mode</pre>	els.huber,	<pre>esmvaltool.diag_scripts.seaborn_diag, 867</pre>
749		<pre>esmvaltool.diag_scripts.shared, 615</pre>
<pre>esmvaltool.diag_scripts.mlr.mode</pre>	els.krr,	<pre>esmvaltool.diag_scripts.shared.iris_helpers,</pre>
757		628
<pre>esmvaltool.diag_scripts.mlr.mode</pre>	els.lasso,	<pre>esmvaltool.diag_scripts.shared.plot,631</pre>
765		itorBase (class in esmval-
esmvaltool.diag_scripts.mlr.mod		tool.diag_scripts.monitor.monitor_base),
773	· ,	844
esmvaltool.diag_scripts.mlr.mod	els.lasso l <b>m</b> org	
781		tool.diag_scripts.ocean.diagnostic_timeseries),

#### 854

854			tool.diag_scripts.mlr.models.linear	r.LinearRegressionModel
<pre>multi_dataset_scatterplot() (in module of </pre>	esmval-		property), 795	-
tool.diag_scripts.shared.plot), 632		numeric	cal_features	(esmval-
<pre>multi_model_contours() (in module of</pre>	esmval-		tool.diag_scripts.mlr.models.linear	r_base.LinearModel
tool.diag_scripts.ocean.diagnostic_map.	<i>s</i> ),		property), 715	
847		numeric	cal_features	(esmval-
	esmval-		tool.diag_scripts.mlr.models.MLR	Model
tool.diag_scripts.ocean.diagnostic_trans	sects),		property), 699	
857		numeric	cal_features	(esmval-
	esmval-		tool.diag_scripts.mlr.models.rfr.RF	FRModel
tool.diag_scripts.ocean.diagnostic_map	os_quad),		property), 803	
848		numeric	cal_features	(esmval-
<pre>multi_model_time_series() (in module of</pre>			tool.diag_scripts.mlr.models.ridge.	RidgeModel
tool.diag_scripts.ocean.diagnostic_time.	eseries),		property), 811	
854		numeric	cal_features	(esmval-
Ν			tool.diag_scripts.mlr.models.ridge_	_cv.RidgeCVModel
			property), 820	
			cal_features	(esmval-
tool.diag_scripts.mlr.custom_sklearn.Aa	lvancedP	ipeline	tool.diag_scripts.mlr.models.svr.SV	/RModel
property), 668			property), 828	
	esmval-	D .		
tool.diag_scripts.mlr.custom_sklearn.Aa	dvancedTi	rdinsforme	dTargetRegressor	
property), 683		pandas_	_object_to_cube() (in modu	
	esmval-		tool.diag_scripts.emergent_constru	uints), 645
tool.diag_scripts.mlr.custom_sklearn.Aa	lvancedP	<i>ipdina</i> met		odels.gbr_base.GBRModel
property), 668	,		property), 707	
numerical_features (e	esmval-	paramet	ers (esmvaltool.diag_scripts.mlr.me	odels.gbr_sklearn.SklearnGBF
tool.diag_scripts.mlr.models.gbr_base.C	JBRMode		property), 724	
property), 707	1	paramet	ers (esmvaltool.diag_scripts.mlr.m.	odels.gbr_xgboost.XGBoostGI
	esmval-	CDDM	property), 732	
tool.diag_scripts.mlr.models.gbr_sklear	n.skiearn	<sup>1</sup> PEFAMea	ers (esmvaltool.diag_scripts.mlr.m	odels.gpr_sklearn.SklearnGPF
property), 724			property), 745	
numerical_features (a	esmvai-	paramet	ers (esmvaltool.diag_scripts.mlr.m	odels.huber.HuberRegressionN
tool.diag_scripts.mlr.models.gbr_xgboo.	SI.AGD00			
property), 732 numerical_features (e	esmval-	paramet	cers (esmvaltool.diag_scripts.mlr.md	odels.krr.KRRModel
		CDDM	property), 762	
tool.diag_scripts.mlr.models.gpr_sklear	n.skiearn	<i>paramea</i>		odels.lasso.LassoModel
property), 745 numerical_features (a	asmual		property), 769	
tool.diag_scripts.mlr.models.huber.Hube	esmval- erPeares	paramet vionModel	cers (esmvaltool.diag_scripts.mlr.md	odels.lasso_cv.LassoCVModel
property), 753	ernegress		1 1 277	
	esmval-	paramet	cers (esmvaltool.diag_scripts.mlr.ma	odels.lasso_lars_cv.LassoLars
tool.diag_scripts.mlr.models.krr.KRRMa			property), 786	- d-l- lin Lin Di l
property), 762	Juei	paramet	cers (esmvaltool.diag_scripts.mlr.m.	oaets.tinear.LinearRegression
	esmval-		property), 795	- d-l- lin M- d-
tool.diag_scripts.mlr.models.lasso.Lasso		paramet	cers (esmvaltool.diag_scripts.mlr.ma	oaeis.iinear_base.LinearMoae
property), 769	mouei		property), 715	- J-1- MIDM - J-1
	esmval-	paramet	ers (esmvaltool.diag_scripts.mlr.m	oaeis.MLRMoaei
tool.diag_scripts.mlr.models.lasso_cv.La		adeh	property), 699	adala ufu DEDMadal
property), 778	ussoc v 111	paramet		oaeis.rjr. <b>kr k</b> moaei
	esmval-	naramo+	property), 803	odals ridaa RidaaMadal
tool.diag_scripts.mlr.models.lasso_lars_		paramet <i>LarsCVM</i>	ers(esmvaltool.diag_scripts.mlr.m Iodelnerty) 811	ouers.ruge.KugeM0aer
property), 786			opfoperty), 811 .ers(esmvaltool.diag_scripts.mlr.m	odals ridge on Pides CVM adal
	esmval-	אמד מווופ נ	property), 820	oueis.riuge_cv.KiugeCviMOuei
(			property), 020	

<pre>parameters(esmvaltool.diag_scripts.mlr.models.svr.SV</pre>		
property), 828	1 - 0	(esmval-
perform_efecv() (in module esmval	<u> </u>	soModel
tool.diag_scripts.mlr.custom_sklearn), 689	method), 770	( 1
-		(esmval-
tool.diag_scripts.mlr.models.gbr_base.GBRMo method), 707	odel tool.diag_scripts.mlr.models.lasso_cv.l method), 778	lassoc v moael
<pre>plot_1d_model() (esmval</pre>	<pre>l- plot_coefs()</pre>	(esmval-
	arnGBRModelool.diag_scripts.mlr.models.lasso_lars	_cv.LassoLarsCVModel
<pre>method), 724 plot_1d_model() (esmval</pre>	<pre>method), 787 l- plot_coefs()</pre>	(esmval-
	BoostGBRModøbl.diag_scripts.mlr.models.linear.Lin	(
method), 733	method), 795	curregressioninouei
		(esmval-
-	arnGPRModelool.diag_scripts.mlr.models.linear_ba	se.LinearModel
method), 745	method), 716	
<pre>plot_1d_model() (esmval</pre>	<pre>l- plot_coefs()</pre>	(esmval-
	ressionModel tool.diag_scripts.mlr.models.ridge.Ridg method), 812	geModel
method), 754 plot_1d_model() (esmval		(esmval-
tool.diag_scripts.mlr.models.krr.KRRModel	tool.diag_scripts.mlr.models.ridge_cv.l	
method), 762	method), 820	
		(esmval-
tool.diag_scripts.mlr.models.lasso.LassoMode		
method), 770	method), 845	
<pre>plot_1d_model() (esmval</pre>	<pre>l- plot_feature_importance()</pre>	(esmval-
tool.diag_scripts.mlr.models.lasso_cv.LassoCV method), 778	VModel tool.diag_scripts.mlr.models.gbr_base. method), 708	GBRModel
		(esmval-
tool.diag_scripts.mlr.models.lasso_lars_cv.Las	ssoLarsCVMotbdl.diag_scripts.mlr.models.gbr_sklea	rn.SklearnGBRModel
<i>method</i> ), 786	<i>method</i> ), 724	
	· · ·	(esmval-
tool.diag_scripts.mlr.models.linear.LinearRegi method), 795	ressionModel tool.diag_scripts.mlr.models.gbr_xgboo method), 733	ost.XGBoostGBRModel
		(esmval-
tool.diag_scripts.mlr.models.linear_base.Linea	arModel tool.diag_scripts.mlr.models.huber.Hul	berRegressionModel
<i>method</i> ), 716	method), 754	
plot_1d_model() (esmval	<pre>l- plot_feature_importance()</pre>	(esmval-
tool.diag_scripts.mlr.models.MLRModel	tool.diag_scripts.mlr.models.lasso.Lass	soModel
method), 699	<i>method</i> ), 770	
plot_1d_model() (esmval	• • •	(esmval-
tool.diag_scripts.mlr.models.rfr.RFRModel method), 803	tool.diag_scripts.mlr.models.lasso_cv.l method), 778	LassoCVModel
<pre>plot_1d_model() (esmval</pre>	<pre>l- plot_feature_importance()</pre>	(esmval-
tool.diag_scripts.mlr.models.ridge.RidgeModel	el tool.diag_scripts.mlr.models.lasso_lars	_cv.LassoLarsCVModel
<i>method</i> ), 812	method), 787	
plot_1d_model() (esmval		(esmval-
tool.diag_scripts.mlr.models.ridge_cv.RidgeCV method), 820	VModel tool.diag_scripts.mlr.models.linear.Lin method), 795	earRegressionModel
plot_1d_model() (esmval		(esmval-
tool.diag_scripts.mlr.models.svr.SVRModel	tool.diag_scripts.mlr.models.linear_ba	•
<pre>method), 828 plot_coefs() (esmval</pre>	<pre>method), 716 l- plot_feature_importance()</pre>	(esmval-
	ressionModel tool.diag_scripts.mlr.models.ridge.Ridg	
vooranas_ser pisininimoueisiniioeniiiioeniii	- content of the set o	

method), 812 plot\_partial\_dependences() (esmvalplot\_feature\_importance() (esmvaltool.diag\_scripts.mlr.models.svr.SVRModel tool.diag scripts.mlr.models.ridge cv.RidgeCVModel method), 829 method), 820 plot\_prediction\_errors() (esmvaltool.diag\_scripts.mlr.models.gbr\_base.GBRModel plot\_individual\_scatterplots() (in module esmvaltool.diag scripts.emergent constraints), method), 708 645 plot\_prediction\_errors() (esmvalplot\_merged\_scatterplots() (in module esmvaltool.diag\_scripts.mlr.models.gbr\_sklearn.SklearnGBRModel tool.diag scripts.emergent constraints), 645 method), 725 plot\_partial\_dependences() (esmval- plot\_prediction\_errors() (esmvaltool.diag\_scripts.mlr.models.gbr\_base.GBRModel tool.diag\_scripts.mlr.models.gbr\_xgboost.XGBoostGBRModel method), 708 method), 733 plot\_partial\_dependences() (esmval- plot\_prediction\_errors() (esmvaltool.diag\_scripts.mlr.models.gbr\_sklearn.SklearnGBRModelool.diag\_scripts.mlr.models.gpr\_sklearn.SklearnGPRModel method), 725 method), 746 plot\_partial\_dependences() (esmval- plot\_prediction\_errors() (esmval $tool.diag\_scripts.mlr.models.gbr\_xgboost.XGBoostGBRModebl.diag\_scripts.mlr.models.huber.HuberRegressionModel$ method), 733 method), 755 plot\_partial\_dependences() (esmval- plot\_prediction\_errors() (esmvaltool.diag scripts.mlr.models.gpr sklearn.SklearnGPRModelool.diag scripts.mlr.models.krr.KRRModel method), 746 method), 762 plot\_partial\_dependences() (esmval- plot\_prediction\_errors() (esmvaltool.diag\_scripts.mlr.models.huber.HuberRegressionModel tool.diag\_scripts.mlr.models.lasso.LassoModel method), 754 method), 771 plot\_partial\_dependences() (*esmval*- plot\_prediction\_errors() (esmvaltool.diag scripts.mlr.models.krr.KRRModel tool.diag\_scripts.mlr.models.lasso\_cv.LassoCVModel method), 762 method), 779 plot\_partial\_dependences() (esmvalplot\_prediction\_errors() (esmvaltool.diag\_scripts.mlr.models.lasso.LassoModel tool.diag\_scripts.mlr.models.lasso\_lars\_cv.LassoLarsCVModel method), 770 method), 787 (esmval- plot\_prediction\_errors() plot\_partial\_dependences() (esmvaltool.diag\_scripts.mlr.models.lasso\_cv.LassoCVModel tool.diag\_scripts.mlr.models.linear.LinearRegressionModel method), 779 method), 796 plot\_partial\_dependences() (esmval- plot\_prediction\_errors() (esmvaltool.diag\_scripts.mlr.models.lasso\_lars\_cv.LassoLarsCVMotbdl.diag\_scripts.mlr.models.linear\_base.LinearModel method), 787 method), 717 plot\_partial\_dependences() (*esmval*- plot\_prediction\_errors() (esmvaltool.diag\_scripts.mlr.models.linear.LinearRegressionModel tool.diag\_scripts.mlr.models.MLRModel method), 796 method), 700 (esmval- plot\_prediction\_errors() plot\_partial\_dependences() (esmvaltool.diag scripts.mlr.models.linear base.LinearModel tool.diag scripts.mlr.models.rfr.RFRModel method), 716 method), 804 plot\_partial\_dependences() (*esmval*- plot\_prediction\_errors() (esmvaltool.diag\_scripts.mlr.models.MLRModel tool.diag\_scripts.mlr.models.ridge.RidgeModel method), 700 method), 813 plot\_partial\_dependences() (esmval- plot\_prediction\_errors() (esmvaltool.diag\_scripts.mlr.models.rfr.RFRModel tool.diag\_scripts.mlr.models.ridge\_cv.RidgeCVModel method), 804 *method*), 821 (esmvalplot\_prediction\_errors() plot\_partial\_dependences() (esmvaltool.diag\_scripts.mlr.models.ridge.RidgeModel tool.diag\_scripts.mlr.models.svr.SVRModel method), 812 method), 829 (esmval- plot\_residuals() plot\_partial\_dependences() (esmvaltool.diag scripts.mlr.models.ridge cv.RidgeCVModel tool.diag scripts.mlr.models.gbr base.GBRModel *method*), 821 method), 708

<pre>plot_residuals()</pre>			esiduals_distribution() lelool.diag_scripts.mlr.models.gpr_skle	(esmval- earn.SklearnGPRModel
method), 725			<i>method</i> ), 746	
<pre>plot_residuals()</pre>	(esmval-	nlot re	esiduals_distribution()	(esmval-
			odebl.diag_scripts.mlr.models.huber.H	
method), 734	0051.1000	05iODIum	method), 755	abernegressionanouei
plot_residuals()	(asmual	nlot r	esiduals_distribution()	(esmval-
		-		
<i>method</i> ), 746			<pre>lelool.diag_scripts.mlr.models.krr.KRR     method), 763</pre>	
<pre>plot_residuals()</pre>			esiduals_distribution()	(esmval-
tool.diag_scripts.mlr.models.huber.H	uberRegres	sionMode	l tool.diag_scripts.mlr.models.lasso.La	ssoModel
method), 755			<i>method</i> ), 771	
<pre>plot_residuals()</pre>	(esmval-	plot_re	esiduals_distribution()	(esmval-
tool.diag_scripts.mlr.models.krr.KRR	Model		tool.diag_scripts.mlr.models.lasso_cv	v.LassoCVModel
<i>method</i> ), 762			<i>method</i> ), 779	
<pre>plot_residuals()</pre>	(esmval-	plot_re	esiduals_distribution()	(esmval-
tool.diag_scripts.mlr.models.lasso.La method), 771	ssoModel		tool.diag_scripts.mlr.models.lasso_la method), 788	rs_cv.LassoLarsCVModel
plot_residuals()	(esmval-	plot_re	esiduals_distribution()	(esmval-
tool.diag_scripts.mlr.models.lasso_cv			tool.diag_scripts.mlr.models.linear.Li	
method), 779			<i>method</i> ), 796	0
<pre>plot_residuals()</pre>	(esmval-	nlot re	esiduals_distribution()	(esmval-
		-	lotball.diag_scripts.mlr.models.linear_b	
method), 788	/5_C/.Eu550		method), 717	use.Emeannouer
plot_residuals()	(esmval_	nlot re	esiduals_distribution()	(esmval-
		-	el tool.diag_scripts.mlr.models.MLRMo	
method), 796	-		method), 700	
<pre>plot_residuals()</pre>			esiduals_distribution()	(esmval-
tool.diag_scripts.mlr.models.linear_b	ase.Linear	Model	tool.diag_scripts.mlr.models.rfr.RFR	Model
<i>method</i> ), 717			<i>method</i> ), 804	
<pre>plot_residuals()</pre>	(esmval-	plot_re	esiduals_distribution()	(esmval-
tool.diag_scripts.mlr.models.MLRMo	del		tool.diag_scripts.mlr.models.ridge.Ri	dgeModel
<i>method</i> ), 700			<i>method</i> ), 813	
<pre>plot_residuals()</pre>	(esmval-	plot_re	esiduals_distribution()	(esmval-
tool.diag_scripts.mlr.models.rfr.RFR method), 804	Model		<pre>tool.diag_scripts.mlr.models.ridge_cv method), 821</pre>	RidgeCVModel
<pre>plot_residuals()</pre>	(esmval-	plot_re	esiduals_distribution()	(esmval-
tool.diag_scripts.mlr.models.ridge.Ri				Model
method), 813	0		method), 829	
<pre>plot_residuals()</pre>	(esmval-	plot re	esiduals_histogram()	(esmval-
tool.diag_scripts.mlr.models.ridge_cv		-	tool.diag_scripts.mlr.models.gbr_bas	
method), 821	11111800071	10000	method), 709	
<pre>plot_residuals()</pre>	(esmval-	nlot re	esiduals_histogram()	(esmval-
tool.diag_scripts.mlr.models.svr.SVR		proc_r	tool.diag_scripts.mlr.models.gbr_skle	
<i>method</i> ), 829			method), 725	
<pre>plot_residuals_distribution()</pre>		-	esiduals_histogram()	(esmval-
tool.diag_scripts.mlr.models.gbr_bas method), 709	e.GBRMod	lel	tool.diag_scripts.mlr.models.gbr_xgb method), 734	oost.XGBoostGBRModel
<pre>plot_residuals_distribution()</pre>	(esmval-	plot_re	esiduals_histogram()	(esmval-
tool.diag_scripts.mlr.models.gbr_skle	earn.Sklear	nGBRMod	lelool.diag_scripts.mlr.models.gpr_skle	earn.SklearnGPRModel
method), 725			<i>method</i> ), 746	
<pre>plot_residuals_distribution()</pre>	(esmval-	plot_re	esiduals_histogram()	(esmval-
		-	odøbl.diag_scripts.mlr.models.huber.H	
<i>method</i> ), 734			<i>method</i> ), 755	0

plot\_residuals\_histogram() (esmval- plot\_scatterplots() (esmvaltool.diag\_scripts.mlr.models.krr.KRRModel tool.diag\_scripts.mlr.models.lasso\_cv.LassoCVModel method), 763 method), 779 plot\_residuals\_histogram() plot\_scatterplots() (esmval-(esmvaltool.diag\_scripts.mlr.models.lasso.LassoModel tool.diag\_scripts.mlr.models.lasso\_lars\_cv.LassoLarsCVModel method), 771 method), 788 plot\_residuals\_histogram() (esmval- plot\_scatterplots() (esmvaltool.diag\_scripts.mlr.models.lasso\_cv.LassoCVModel tool.diag\_scripts.mlr.models.linear.LinearRegressionModel method), 779 method), 796 (esmval- plot\_scatterplots() plot\_residuals\_histogram() (esmvaltool.diag\_scripts.mlr.models.lasso\_lars\_cv.LassoLarsCVMotbdl.diag\_scripts.mlr.models.linear\_base.LinearModel method), 788 method), 717 plot\_residuals\_histogram() (esmval- plot\_scatterplots() (esmvaltool.diag\_scripts.mlr.models.linear.LinearRegressionModel tool.diag\_scripts.mlr.models.MLRModel method), 796 *method*), 701 plot\_residuals\_histogram() (esmval- plot\_scatterplots() (esmvaltool.diag\_scripts.mlr.models.linear\_base.LinearModel tool.diag\_scripts.mlr.models.rfr.RFRModel method), 717 method), 805 plot\_residuals\_histogram() (esmval- plot\_scatterplots() (esmvaltool.diag scripts.mlr.models.ridge.RidgeModel tool.diag scripts.mlr.models.MLRModel method), 700 *method*), 813 plot\_residuals\_histogram() (esmval- plot\_scatterplots() (esmvaltool.diag\_scripts.mlr.models.rfr.RFRModel tool.diag\_scripts.mlr.models.ridge\_cv.RidgeCVModel method). 804 method). 821 plot\_residuals\_histogram() (esmvalplot\_scatterplots() (esmvaltool.diag\_scripts.mlr.models.ridge.RidgeModel tool.diag\_scripts.mlr.models.svr.SVRModel method), 813 method), 830 plot\_residuals\_histogram() (esmval- plot\_target\_distributions() (in module esmvaltool.diag\_scripts.mlr.models.ridge\_cv.RidgeCVModel tool.diag\_scripts.emergent\_constraints), 646 method), 821 plot\_timeseries() (esmvalplot\_residuals\_histogram() tool.diag\_scripts.monitor.monitor\_base.MonitorBase (esmvaltool.diag\_scripts.mlr.models.svr.SVRModel method), 845 method), 829 plot\_training\_progress() (esmvalplot\_scatterplots() (esmvaltool.diag\_scripts.mlr.models.gbr\_sklearn.SklearnGBRModel tool.diag\_scripts.mlr.models.gbr\_base.GBRModel method), 726 method), 709 plot\_training\_progress() (esmvalplot\_scatterplots() (esmvaltool.diag scripts.mlr.models.gbr xgboost.XGBoostGBRModel tool.diag\_scripts.mlr.models.gbr\_sklearn.SklearnGBRModelnethod), 734 method), 725 predict() (esmvaltool.diag\_scripts.mlr.custom\_sklearn.AdvancedPipeline plot\_scatterplots() (esmvalmethod), 668 tool.diag scripts.mlr.models.gbr xgboost.XGBoospGBRMtoQp((esmvaltool.diag scripts.mlr.custom sklearn.AdvancedRFE method), 734 method), 675 plot\_scatterplots() (esmval- predict() (esmvaltool.diag\_scripts.mlr.custom\_sklearn.AdvancedRFECV  $tool. diag\_scripts.mlr.models.gpr\_sklearn.SklearnGPRModelmethod), 679$ method), 747 predict() (esmvaltool.diag\_scripts.mlr.custom\_sklearn.AdvancedTransfor plot\_scatterplots() method), 683 (esmvaltool.diag\_scripts.mlr.models.huber.HuberRegressipnetCidet() (esmvaltool.diag\_scripts.mlr.models.gbr\_base.GBRModel method), 755 method), 709 (esmvalplot\_scatterplots() predict() (esmvaltool.diag\_scripts.mlr.models.gbr\_sklearn.SklearnGBRM tool.diag\_scripts.mlr.models.krr.KRRModel method), 726 method), 763 predict() (esmvaltool.diag\_scripts.mlr.models.gbr\_xgboost.XGBoostGBH method), 734 plot\_scatterplots() (esmvaltool.diag scripts.mlr.models.lasso.LassoModel predict() (esmvaltool.diag\_scripts.mlr.models.gpr\_sklearn.AdvancedGau method), 771 method), 738

#### ESMValTool User's and Developer's Guide, Release 2.11.0.dev52+g696097c.d20240424

	() (esmvaltool.diag_scripts.mlr.models.gp method), 747		6 <b>iff@Maxi</b> &on_matrices() tool.diag_scripts.mlr.models.gbr_xgbo	(esmval-
				osi.AODoosiODKmodei
	() (esmvaltool.diag_scripts.mlr.models.hu method), 755			(esmval-
	() (esmvaltool.diag_scripts.mlr.models.kri	-	tool.diag_scripts.mlr.models.gpr_sklea	
-	method), 763		method), 747	in.skicamor Kinbaci
	() (esmvaltool.diag_scripts.mlr.models.las			(esmval-
	method), 771		tool.diag_scripts.mlr.models.huber.Hu	
	() (esmvaltool.diag_scripts.mlr.models.las			bernegressionmouer
	method), 780			(esmval-
	() (esmvaltool.diag_scripts.mlr.models.las	-		•
-	method), 788		method), 764	Iouci
	() (esmvaltool.diag_scripts.mlr.models.lin			(esmval-
	method), 797	-	tool.diag_scripts.mlr.models.lasso.Las	
	() (esmvaltool.diag_scripts.mlr.models.lin		~ ·	somouer
	method), 717			(esmval-
	() (esmvaltool.diag_scripts.mlr.models.Ml		tool.diag_scripts.mlr.models.lasso_cv.	
	method), 701		method), 780	LussoC v model
	() (esmvaltool.diag_scripts.mlr.models.rfr			(esmval-
	method), 805		tool.diag_scripts.mlr.models.lasso_lar	
	() (esmvaltool.diag_scripts.mlr.models.ria			s_cv.LassoLarsCvmodel
-	· · · · ·			( agreed al
	method), 813	-		(esmval-
	() (esmvaltool.diag_scripts.mlr.models.ria			iearRegressionMoaei
	method), 822		method), 797	( agreed al
	() (esmvaltool.diag_scripts.mlr.models.svi			(esmval-
	method), 830		tool.diag_scripts.mlr.models.linear_ba	ise.LinearMoael
-			method), 718	( 1
	tool.diag_scripts.mlr.custom_sklearn.Adv	-		(esmval-
	<i>method</i> ), 669		tool.diag_scripts.mlr.models.MLRMod	lel
-			method), 701	/ I
	tool.diag_scripts.mlr.custom_sklearn.Adv			(esmval-
	<i>method</i> ), 675		tool.diag_scripts.mlr.models.rfr.RFRM	lodel
-			method), 805	, .
	tool.diag_scripts.mlr.custom_sklearn.Adv	-		(esmval-
	method), 680		tool.diag_scripts.mlr.models.ridge.Rid	geModel
predict_	$\operatorname{proha}()$ (es			0
	-		<i>method</i> ), 814	-
	tool.diag_scripts.mlr.custom_sklearn.Adv	vancedPi <b>pedim</b> et_co	<pre>method), 814 orrelation_matrices()</pre>	(esmval-
	tool.diag_scripts.mlr.custom_sklearn.Adv method), 670	vancedPi <b>pedim</b> et_co	<pre>method), 814 orrelation_matrices() tool.diag_scripts.mlr.models.ridge_cv</pre>	(esmval-
predict_	tool.diag_scripts.mlr.custom_sklearn.Adv method), 670 _proba() (es	vancedPi <b>pedim</b> t_co smval-	<pre>method), 814 orrelation_matrices() tool.diag_scripts.mlr.models.ridge_cv method), 822</pre>	(esmval- RidgeCVModel
predict_	tool.diag_scripts.mlr.custom_sklearn.Adv method), 670 _proba() (es tool.diag_scripts.mlr.custom_sklearn.Adv	vancedPi <b>pedimet_co</b> smval- vancedRFAFrint_co	<pre>method), 814 orrelation_matrices() tool.diag_scripts.mlr.models.ridge_cv method), 822 orrelation_matrices()</pre>	(esmval- RidgeCVModel (esmval-
predict_	tool.diag_scripts.mlr.custom_sklearn.Adv method), 670 _proba() (es tool.diag_scripts.mlr.custom_sklearn.Adv method), 675	vancedPi <b>pedime</b> t_co smval- vancedRF#rint_co	<pre>method), 814 orrelation_matrices() tool.diag_scripts.mlr.models.ridge_cv method), 822 orrelation_matrices() tool.diag_scripts.mlr.models.svr.SVRM</pre>	(esmval- RidgeCVModel (esmval-
predict_ predict_	tool.diag_scripts.mlr.custom_sklearn.Adv method), 670 _proba() (es tool.diag_scripts.mlr.custom_sklearn.Adv method), 675 _proba() (es	vancedPi <b>pedime</b> t_co smval- vanced <b>RFfFrint_co</b> smval-	<pre>method), 814 orrelation_matrices() tool.diag_scripts.mlr.models.ridge_cv method), 822 orrelation_matrices() tool.diag_scripts.mlr.models.svr.SVRM method), 830</pre>	(esmval- RidgeCVModel (esmval- lodel
predict_ predict_	tool.diag_scripts.mlr.custom_sklearn.Adv method), 670 _proba() (es tool.diag_scripts.mlr.custom_sklearn.Adv method), 675 _proba() (es tool.diag_scripts.mlr.custom_sklearn.Adv	vancedPi <b>palim</b> e_co smval- vancedRFfFrint_co smval- vancedRFfFGWt_ko	<pre>method), 814 orrelation_matrices() tool.diag_scripts.mlr.models.ridge_cv method), 822 orrelation_matrices() tool.diag_scripts.mlr.models.svr.SVRM method), 830 ernel_info()</pre>	(esmval- RidgeCVModel (esmval- lodel (esmval-
predict_ predict_	tool.diag_scripts.mlr.custom_sklearn.Adv method), 670 _proba() (es tool.diag_scripts.mlr.custom_sklearn.Adv method), 675 _proba() (es tool.diag_scripts.mlr.custom_sklearn.Adv method), 680	vancedPi <b>palim</b> t_co smval- vancedRFfFrint_co smval- vancedRFfFCHt_ko	<pre>method), 814 orrelation_matrices() tool.diag_scripts.mlr.models.ridge_cv method), 822 orrelation_matrices() tool.diag_scripts.mlr.models.svr.SVRM method), 830 ernel_info() tool.diag_scripts.mlr.models.gpr_skled</pre>	(esmval- RidgeCVModel (esmval- lodel (esmval-
predict_ predict_ prepare_	tool.diag_scripts.mlr.custom_sklearn.Adv method), 670 _proba() (es tool.diag_scripts.mlr.custom_sklearn.Adv method), 675 _proba() (es tool.diag_scripts.mlr.custom_sklearn.Adv method), 680 _cube_for_merging() (in module es	vancedPi <b>palim</b> t_co smval- vancedRFfFrint_co smval- vancedRFfFGHt_ko smval-	<pre>method), 814 orrelation_matrices() tool.diag_scripts.mlr.models.ridge_cv method), 822 orrelation_matrices() tool.diag_scripts.mlr.models.svr.SVRM method), 830 ernel_info() tool.diag_scripts.mlr.models.gpr_skled method), 748</pre>	(esmval- RidgeCVModel (esmval- lodel (esmval-
predict_ predict_ prepare_	tool.diag_scripts.mlr.custom_sklearn.Adv method), 670 _proba() (es tool.diag_scripts.mlr.custom_sklearn.Adv method), 675 _proba() (es tool.diag_scripts.mlr.custom_sklearn.Adv method), 680 _cube_for_merging() (in module es tool.diag_scripts.shared.iris_helpers), 630	vancedPi <b>pedimet_co</b> smval- vancedRFffrint_co smval- vancedRFffrGWt_ko smval- 0 print_ro	<pre>method), 814 orrelation_matrices() tool.diag_scripts.mlr.models.ridge_cv method), 822 orrelation_matrices() tool.diag_scripts.mlr.models.svr.SVRM method), 830 ernel_info() tool.diag_scripts.mlr.models.gpr_skled method), 748 egression_metrics()</pre>	(esmval- RidgeCVModel (esmval- lodel (esmval- ırn.SklearnGPRModel (esmval-
predict_ predict_ prepare_ prepare_	tool.diag_scripts.mlr.custom_sklearn.Adv method), 670 _proba() (es tool.diag_scripts.mlr.custom_sklearn.Adv method), 675 _proba() (es tool.diag_scripts.mlr.custom_sklearn.Adv method), 680 _cube_for_merging() (in module es tool.diag_scripts.shared.iris_helpers), 630 _provenance_record() (in module es	vancedPi <b>pedimet_co</b> smval- vancedRFfFrint_co smval- vancedRFfFCWt_ko smval- 0 print_ro smval-	<pre>method), 814 orrelation_matrices() tool.diag_scripts.mlr.models.ridge_cv method), 822 orrelation_matrices() tool.diag_scripts.mlr.models.svr.SVRM method), 830 ernel_info() tool.diag_scripts.mlr.models.gpr_skled method), 748 egression_metrics() tool.diag_scripts.mlr.models.gbr_base</pre>	(esmval- RidgeCVModel (esmval- lodel (esmval- ırn.SklearnGPRModel (esmval-
predict_ predict_ prepare_ prepare_	tool.diag_scripts.mlr.custom_sklearn.Adv method), 670 _proba() (es tool.diag_scripts.mlr.custom_sklearn.Adv method), 675 _proba() (es tool.diag_scripts.mlr.custom_sklearn.Adv method), 680 _cube_for_merging() (in module es tool.diag_scripts.shared.iris_helpers), 630 _provenance_record() (in module es tool.diag_scripts.ocean.diagnostic_tools);	vancedPi <b>pedimet_</b> co smval- vancedRFffrint_co smval- vancedRFfffCWt_ko smval- 0 print_ro smval- 0, 866	<pre>method), 814 orrelation_matrices() tool.diag_scripts.mlr.models.ridge_cv method), 822 orrelation_matrices() tool.diag_scripts.mlr.models.svr.SVRM method), 830 ernel_info() tool.diag_scripts.mlr.models.gpr_skled method), 748 egression_metrics() tool.diag_scripts.mlr.models.gbr_base method), 710</pre>	(esmval- RidgeCVModel (esmval- lodel (esmval- ırn.SklearnGPRModel (esmval-
predict_ predict_ prepare_ prepare_ print_cc	tool.diag_scripts.mlr.custom_sklearn.Adv method), 670 _proba() (es tool.diag_scripts.mlr.custom_sklearn.Adv method), 675 _proba() (es tool.diag_scripts.mlr.custom_sklearn.Adv method), 680 _cube_for_merging() (in module es tool.diag_scripts.shared.iris_helpers), 630 _provenance_record() (in module es tool.diag_scripts.ocean.diagnostic_tools). prrelation_matrices() (es	vancedPi <b>palim</b> t_co smval- vancedRFfFrint_co smval- vancedRFfFCWt_ko smval- 0 print_ro smval- 0, 866 smval- print_ro	<pre>method), 814 orrelation_matrices() tool.diag_scripts.mlr.models.ridge_cv method), 822 orrelation_matrices() tool.diag_scripts.mlr.models.svr.SVRM method), 830 ernel_info() tool.diag_scripts.mlr.models.gpr_skled method), 748 egression_metrics() tool.diag_scripts.mlr.models.gbr_base method), 710 egression_metrics()</pre>	(esmval- RidgeCVModel (esmval- lodel (esmval- urn.SklearnGPRModel (esmval- .GBRModel (esmval-
predict_ predict_ prepare_ prepare_ print_co	tool.diag_scripts.mlr.custom_sklearn.Adv method), 670 _proba() (es tool.diag_scripts.mlr.custom_sklearn.Adv method), 675 _proba() (es tool.diag_scripts.mlr.custom_sklearn.Adv method), 680 _cube_for_merging() (in module es tool.diag_scripts.shared.iris_helpers), 630 _provenance_record() (in module es tool.diag_scripts.ocean.diagnostic_tools). prrelation_matrices() (es tool.diag_scripts.mlr.models.gbr_base.GB	vancedPi <b>palim</b> t_co smval- vancedRFfFrint_co smval- vancedRFfFCWt_ko smval- 0 print_ro smval- 0, 866 smval- print_ro BRModel	<pre>method), 814 orrelation_matrices() tool.diag_scripts.mlr.models.ridge_cv method), 822 orrelation_matrices() tool.diag_scripts.mlr.models.svr.SVRM method), 830 ernel_info() tool.diag_scripts.mlr.models.gpr_skled method), 748 egression_metrics() tool.diag_scripts.mlr.models.gbr_base method), 710 egression_metrics() tool.diag_scripts.mlr.models.gbr_skled method), 710</pre>	(esmval- RidgeCVModel (esmval- lodel (esmval- urn.SklearnGPRModel (esmval- .GBRModel (esmval-
predict_ predict_ prepare_ prepare_ print_co	tool.diag_scripts.mlr.custom_sklearn.Adv method), 670 _proba() (es tool.diag_scripts.mlr.custom_sklearn.Adv method), 675 _proba() (es tool.diag_scripts.mlr.custom_sklearn.Adv method), 680 _cube_for_merging() (in module es tool.diag_scripts.shared.iris_helpers), 630 _provenance_record() (in module es tool.diag_scripts.ocean.diagnostic_tools) prrelation_matrices() (es tool.diag_scripts.mlr.models.gbr_base.Gb method), 710	vancedPi <b>palim</b> t_co smval- vancedRFfFrint_co smval- vancedRFfFGWt_ko smval- 0 print_ro smval- 0, 866 smval- print_ro BRModel	<pre>method), 814 orrelation_matrices() tool.diag_scripts.mlr.models.ridge_cv method), 822 orrelation_matrices() tool.diag_scripts.mlr.models.svr.SVRM method), 830 ernel_info() tool.diag_scripts.mlr.models.gpr_skled method), 748 egression_metrics() tool.diag_scripts.mlr.models.gbr_base method), 710 egression_metrics() tool.diag_scripts.mlr.models.gbr_skled method), 726</pre>	(esmval- RidgeCVModel (esmval- lodel (esmval- urn.SklearnGPRModel (esmval- .GBRModel (esmval- urn.SklearnGBRModel
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print_regression_metrics() (esmval- random tool diag. scripts mlr models apr. sklearn Sklearn GPRM	delool.diag_scripts.mlr.models.gbr_xgboost.XGBoostGBRModel
method), 748	property), 735
print_regression_metrics() (esmval- random	
	el tool.diag_scripts.mlr.models.gpr_sklearn.SklearnGPRModel
method), 756	property), 748
print_regression_metrics() (esmval- random	
tool.diag_scripts.mlr.models.krr.KRRModel	tool.diag_scripts.mlr.models.huber.HuberRegressionModel
method), 764	property), 756
print_regression_metrics() (esmval- random	
tool.diag_scripts.mlr.models.lasso.LassoModel	tool.diag_scripts.mlr.models.krr.KRRModel
method), 772	property), 764
<pre>print_regression_metrics() (esmval- random</pre>	
tool.diag_scripts.mlr.models.lasso_cv.LassoCVModel	tool.diag_scripts.mlr.models.lasso.LassoModel
method), 780	property), 772
<pre>print_regression_metrics() (esmval- random</pre>	n_state (esmval-
tool.diag_scripts.mlr.models.lasso_lars_cv.LassoLarsCV	Motball.diag_scripts.mlr.models.lasso_cv.LassoCVModel
method), 789	property), 780
<pre>print_regression_metrics() (esmval- random</pre>	
	lel tool.diag_scripts.mlr.models.lasso_lars_cv.LassoLarsCVModel
method), 797	property), 789
<pre>print_regression_metrics() (esmval- random</pre>	
tool.diag_scripts.mlr.models.linear_base.LinearModel	
method), 718	property), 797
print_regression_metrics() (esmval- random	
tool.diag_scripts.mlr.models.MLRModel method), 702	tool.diag_scripts.mlr.models.linear_base.LinearModel property), 718
<pre>print_regression_metrics() (esmval- random </pre>	
tool.diag_scripts.mlr.models.rfr.RFRModel	tool.diag_scripts.mlr.models.MLRModel
tool.diag_scripts.mlr.models.rfr.RFRModel method), 806	tool.diag_scripts.mlr.models.MLRModel property), 702
<pre>tool.diag_scripts.mlr.models.rfr.RFRModel     method), 806 print_regression_metrics() (esmval- random</pre>	tool.diag_scripts.mlr.models.MLRModel property), 702 _state (esmval-
<pre>tool.diag_scripts.mlr.models.rfr.RFRModel     method), 806 print_regression_metrics() (esmval- random     tool.diag_scripts.mlr.models.ridge.RidgeModel</pre>	tool.diag_scripts.mlr.models.MLRModel property), 702 state (esmval- tool.diag_scripts.mlr.models.rfr.RFRModel
<pre>tool.diag_scripts.mlr.models.rfr.RFRModel     method), 806 print_regression_metrics() (esmval- random     tool.diag_scripts.mlr.models.ridge.RidgeModel     method), 814</pre>	tool.diag_scripts.mlr.models.MLRModel property), 702 state (esmval- tool.diag_scripts.mlr.models.rfr.RFRModel property), 806
<pre>tool.diag_scripts.mlr.models.rfr.RFRModel     method), 806 print_regression_metrics() (esmval-     tool.diag_scripts.mlr.models.ridge.RidgeModel     method), 814 print_regression_metrics() (esmval-     random </pre>	tool.diag_scripts.mlr.models.MLRModel property), 702 state (esmval- tool.diag_scripts.mlr.models.rfr.RFRModel property), 806 state (esmval-
<pre>tool.diag_scripts.mlr.models.rfr.RFRModel     method), 806 print_regression_metrics() (esmval- random     tool.diag_scripts.mlr.models.ridge.RidgeModel     method), 814 print_regression_metrics() (esmval- random     tool.diag_scripts.mlr.models.ridge_cv.RidgeCVModel     method), 822</pre>	tool.diag_scripts.mlr.models.MLRModel property), 702 state (esmval- tool.diag_scripts.mlr.models.rfr.RFRModel property), 806 state (esmval- tool.diag_scripts.mlr.models.ridge.RidgeModel property), 814
<pre>tool.diag_scripts.mlr.models.rfr.RFRModel     method), 806 print_regression_metrics() (esmval- random     tool.diag_scripts.mlr.models.ridge.RidgeModel     method), 814 print_regression_metrics() (esmval- random     tool.diag_scripts.mlr.models.ridge_cv.RidgeCVModel     method), 822 print_regression_metrics() (esmval- random     rando</pre>	tool.diag_scripts.mlr.models.MLRModel property), 702 _state (esmval- tool.diag_scripts.mlr.models.rfr.RFRModel property), 806 _state (esmval- tool.diag_scripts.mlr.models.ridge.RidgeModel property), 814 _state (esmval-
<pre>tool.diag_scripts.mlr.models.rfr.RFRModel     method), 806 print_regression_metrics() (esmval- random     tool.diag_scripts.mlr.models.ridge.RidgeModel     method), 814 print_regression_metrics() (esmval- random     tool.diag_scripts.mlr.models.ridge_cv.RidgeCVModel     method), 822 print_regression_metrics() (esmval- random     tool.diag_scripts.mlr.models.svr.SVRModel</pre>	tool.diag_scripts.mlr.models.MLRModel property), 702 state (esmval- tool.diag_scripts.mlr.models.rfr.RFRModel property), 806 state (esmval- tool.diag_scripts.mlr.models.ridge.RidgeModel property), 814 state (esmval- tool.diag_scripts.mlr.models.ridge_cv.RidgeCVModel
<pre>tool.diag_scripts.mlr.models.rfr.RFRModel     method), 806 print_regression_metrics() (esmval- random     tool.diag_scripts.mlr.models.ridge.RidgeModel     method), 814 print_regression_metrics() (esmval- random     tool.diag_scripts.mlr.models.ridge_cv.RidgeCVModel     method), 822 print_regression_metrics() (esmval- random     tool.diag_scripts.mlr.models.svr.SVRModel     method), 831</pre>	tool.diag_scripts.mlr.models.MLRModel property), 702 state (esmval- tool.diag_scripts.mlr.models.rfr.RFRModel property), 806 state (esmval- tool.diag_scripts.mlr.models.ridge.RidgeModel property), 814 state (esmval- tool.diag_scripts.mlr.models.ridge_cv.RidgeCVModel property), 822
<pre>tool.diag_scripts.mlr.models.rfr.RFRModel method), 806 print_regression_metrics() (esmval- random tool.diag_scripts.mlr.models.ridge.RidgeModel method), 814 print_regression_metrics() (esmval- random tool.diag_scripts.mlr.models.ridge_cv.RidgeCVModel method), 822 print_regression_metrics() (esmval- random tool.diag_scripts.mlr.models.svr.SVRModel method), 831 ProvenanceLogger (class in esmval- random)</pre>	tool.diag_scripts.mlr.models.MLRModel property), 702 state (esmval- tool.diag_scripts.mlr.models.rfr.RFRModel property), 806 state (esmval- tool.diag_scripts.mlr.models.ridge.RidgeModel property), 814 state (esmval- tool.diag_scripts.mlr.models.ridge_cv.RidgeCVModel property), 822 state (esmval-
<pre>tool.diag_scripts.mlr.models.rfr.RFRModel     method), 806 print_regression_metrics() (esmval- random     tool.diag_scripts.mlr.models.ridge.RidgeModel     method), 814 print_regression_metrics() (esmval- random     tool.diag_scripts.mlr.models.ridge_cv.RidgeCVModel     method), 822 print_regression_metrics() (esmval- random     tool.diag_scripts.mlr.models.svr.SVRModel     method), 831</pre>	tool.diag_scripts.mlr.models.MLRModel property), 702 state (esmval- tool.diag_scripts.mlr.models.rfr.RFRModel property), 806 state (esmval- tool.diag_scripts.mlr.models.ridge.RidgeModel property), 814 state (esmval- tool.diag_scripts.mlr.models.ridge_cv.RidgeCVModel property), 822 state (esmval- tool.diag_scripts.mlr.models.svr.SVRModel
<pre>tool.diag_scripts.mlr.models.rfr.RFRModel     method), 806 print_regression_metrics() (esmval- random     tool.diag_scripts.mlr.models.ridge.RidgeModel     method), 814 print_regression_metrics() (esmval- random     tool.diag_scripts.mlr.models.ridge_cv.RidgeCVModel     method), 822 print_regression_metrics() (esmval- random     tool.diag_scripts.mlr.models.svr.SVRModel     method), 831 ProvenanceLogger (class in esmval- random     tool.diag_scripts.shared), 620</pre>	tool.diag_scripts.mlr.models.MLRModel property), 702 _state (esmval- tool.diag_scripts.mlr.models.rfr.RFRModel property), 806 _state (esmval- tool.diag_scripts.mlr.models.ridge.RidgeModel property), 814 _state (esmval- tool.diag_scripts.mlr.models.ridge_cv.RidgeCVModel property), 822 _state (esmval- tool.diag_scripts.mlr.models.svr.SVRModel property), 831
<pre>tool.diag_scripts.mlr.models.rfr.RFRModel     method), 806 print_regression_metrics() (esmval- random     tool.diag_scripts.mlr.models.ridge.RidgeModel     method), 814 print_regression_metrics() (esmval- random     tool.diag_scripts.mlr.models.ridge_cv.RidgeCVModel     method), 822 print_regression_metrics() (esmval- random     tool.diag_scripts.mlr.models.svr.SVRModel     method), 831 ProvenanceLogger (class in esmval- random     tool.diag_scripts.shared), 620 </pre>	tool.diag_scripts.mlr.models.MLRModel property), 702 state (esmval- tool.diag_scripts.mlr.models.rfr.RFRModel property), 806 state (esmval- tool.diag_scripts.mlr.models.ridge.RidgeModel property), 814 state (esmval- tool.diag_scripts.mlr.models.ridge_cv.RidgeCVModel property), 822 state (esmval- tool.diag_scripts.mlr.models.svr.SVRModel property), 831 L_plot_provenance() (esmval-
<pre>tool.diag_scripts.mlr.models.rfr.RFRModel     method), 806 print_regression_metrics() (esmval- random     tool.diag_scripts.mlr.models.ridge.RidgeModel     method), 814 print_regression_metrics() (esmval- random     tool.diag_scripts.mlr.models.ridge_cv.RidgeCVModel     method), 822 print_regression_metrics() (esmval- random     tool.diag_scripts.mlr.models.svr.SVRModel     method), 831 ProvenanceLogger (class in esmval- random     tool.diag_scripts.shared), 620 Q record quickplot() (in module esmval-</pre>	tool.diag_scripts.mlr.models.MLRModel property), 702 state (esmval- tool.diag_scripts.mlr.models.rfr.RFRModel property), 806 state (esmval- tool.diag_scripts.mlr.models.ridge.RidgeModel property), 814 state (esmval- tool.diag_scripts.mlr.models.ridge_cv.RidgeCVModel property), 822 state (esmval- tool.diag_scripts.mlr.models.svr.SVRModel property), 831 Lplot_provenance() (esmval- tool.diag_scripts.monitor.monitor_base.MonitorBase
<pre>tool.diag_scripts.mlr.models.rfr.RFRModel     method), 806 print_regression_metrics() (esmval- random     tool.diag_scripts.mlr.models.ridge.RidgeModel     method), 814 print_regression_metrics() (esmval- random     tool.diag_scripts.mlr.models.ridge_cv.RidgeCVModel     method), 822 print_regression_metrics() (esmval- random     tool.diag_scripts.mlr.models.svr.SVRModel     method), 831 ProvenanceLogger (class in esmval- random     tool.diag_scripts.shared), 620 Q record quickplot() (in module esmval-     tool.diag_scripts.shared.plot), 633</pre>	tool.diag_scripts.mlr.models.MLRModel property), 702 state (esmval- tool.diag_scripts.mlr.models.rfr.RFRModel property), 806 state (esmval- tool.diag_scripts.mlr.models.ridge.RidgeModel property), 814 state (esmval- tool.diag_scripts.mlr.models.ridge_cv.RidgeCVModel property), 822 state (esmval- tool.diag_scripts.mlr.models.svr.SVRModel property), 831 L_plot_provenance() (esmval-
<pre>tool.diag_scripts.mlr.models.rfr.RFRModel     method), 806 print_regression_metrics() (esmval- random     tool.diag_scripts.mlr.models.ridge.RidgeModel     method), 814 print_regression_metrics() (esmval- random     tool.diag_scripts.mlr.models.ridge_cv.RidgeCVModel     method), 822 print_regression_metrics() (esmval- random     tool.diag_scripts.mlr.models.svr.SVRModel     method), 831 ProvenanceLogger (class in esmval-     tool.diag_scripts.shared), 620 Q record quickplot() (in module esmval-     tool.diag_scripts.shared.plot), 633 regist</pre>	tool.diag_scripts.mlr.models.MLRModel property), 702 state (esmval- tool.diag_scripts.mlr.models.rfr.RFRModel property), 806 state (esmval- tool.diag_scripts.mlr.models.ridge.RidgeModel property), 814 state (esmval- tool.diag_scripts.mlr.models.ridge_cv.RidgeCVModel property), 822 state (esmval- tool.diag_scripts.mlr.models.svr.SVRModel property), 831 plot_provenance() (esmval- tool.diag_scripts.monitor.monitor_base.MonitorBase method), 845
<pre>tool.diag_scripts.mlr.models.rfr.RFRModel     method), 806 print_regression_metrics() (esmval- random     tool.diag_scripts.mlr.models.ridge.RidgeModel     method), 814 print_regression_metrics() (esmval- random     tool.diag_scripts.mlr.models.ridge_cv.RidgeCVModel     method), 822 print_regression_metrics() (esmval- random     tool.diag_scripts.mlr.models.svr.SVRModel     method), 831 ProvenanceLogger (class in esmval-     random     tool.diag_scripts.shared), 620 Q record quickplot() (in module esmval-     tool.diag_scripts.shared.plot), 633 R mandem state</pre>	tool.diag_scripts.mlr.models.MLRModel property), 702 state (esmval- tool.diag_scripts.mlr.models.rfr.RFRModel property), 806 state (esmval- tool.diag_scripts.mlr.models.ridge.RidgeModel property), 814 state (esmval- tool.diag_scripts.mlr.models.ridge_cv.RidgeCVModel property), 822 state (esmval- tool.diag_scripts.mlr.models.svr.SVRModel property), 831 L_plot_provenance() (esmval- tool.diag_scripts.monitor.monitor_base.MonitorBase method), 845 :er_mlr_model() (esmval- tool.diag_scripts.mlr.models.gbr_base.GBRModel class method), 710
<pre>tool.diag_scripts.mlr.models.rfr.RFRModel     method), 806 print_regression_metrics() (esmval- random     tool.diag_scripts.mlr.models.ridge.RidgeModel     method), 814 print_regression_metrics() (esmval- random     tool.diag_scripts.mlr.models.ridge_cv.RidgeCVModel     method), 822 print_regression_metrics() (esmval- random     tool.diag_scripts.mlr.models.svr.SVRModel     method), 831 ProvenanceLogger (class in esmval-     random     tool.diag_scripts.shared), 620 Q record quickplot() (in module esmval-     tool.diag_scripts.shared.plot), 633 R mandem state</pre>	<pre>tool.diag_scripts.mlr.models.MLRModel property), 702state (esmval- tool.diag_scripts.mlr.models.rfr.RFRModel property), 806state (esmval- tool.diag_scripts.mlr.models.ridge.RidgeModel property), 814state (esmval- tool.diag_scripts.mlr.models.ridge_cv.RidgeCVModel property), 822state (esmval- tool.diag_scripts.mlr.models.svr.SVRModel property), 831 L_plot_provenance() (esmval- tool.diag_scripts.monitor.monitor_base.MonitorBase method), 845 :er_mlr_model() (esmval- tool.diag_scripts.mlr.models.gbr_base.GBRModel class method), 710 :er_mlr_model() (esmval- </pre>
<pre>tool.diag_scripts.mlr.models.rfr.RFRModel     method), 806 print_regression_metrics() (esmval- random     tool.diag_scripts.mlr.models.ridge_RidgeModel     method), 814 print_regression_metrics() (esmval- random     tool.diag_scripts.mlr.models.ridge_cv.RidgeCVModel     method), 822 print_regression_metrics() (esmval- random     tool.diag_scripts.mlr.models.svr.SVRModel     method), 831 ProvenanceLogger (class in esmval- random     tool.diag_scripts.shared), 620 Q record quickplot() (in module esmval-     tool.diag_scripts.shared.plot), 633 R random_state (esmval-     tool.diag_scripts.mlr.models.gbr_base.GBRModel regist </pre>	<pre>tool.diag_scripts.mlr.models.MLRModel property), 702state (esmval- tool.diag_scripts.mlr.models.rfr.RFRModel property), 806state (esmval- tool.diag_scripts.mlr.models.ridge_CVModel property), 814state (esmval- tool.diag_scripts.mlr.models.svr.SVRModel property), 822state (esmval- tool.diag_scripts.mlr.models.svr.SVRModel property), 831 L_plot_provenance() (esmval- tool.diag_scripts.monitor.monitor_base.MonitorBase method), 845 ser_mlr_model() (esmval- tool.diag_scripts.mlr.models.gbr_base.GBRModel class method), 710 ser_mlr_model() (esmval- tool.diag_scripts.mlr.models.gbr_sklearn.SklearnGBRModel</pre>
<pre>tool.diag_scripts.mlr.models.rfr.RFRModel     method), 806 print_regression_metrics() (esmval- random     tool.diag_scripts.mlr.models.ridge.RidgeModel     method), 814 print_regression_metrics() (esmval- random     tool.diag_scripts.mlr.models.ridge_cv.RidgeCVModel     method), 822 print_regression_metrics() (esmval- random     tool.diag_scripts.mlr.models.svr.SVRModel     method), 831 ProvenanceLogger (class in esmval- random     tool.diag_scripts.shared), 620 Q record quickplot() (in module esmval-     tool.diag_scripts.shared.plot), 633 R random_state (esmval-     tool.diag_scripts.mlr.models.gbr_base.GBRModel     regiss     property), 710 random ctate     (asmval-</pre>	<pre>tool.diag_scripts.mlr.models.MLRModel property), 702state (esmval- tool.diag_scripts.mlr.models.rfr.RFRModel property), 806state (esmval- tool.diag_scripts.mlr.models.ridge_CVModel property), 814state (esmval- tool.diag_scripts.mlr.models.svr.SVRModel property), 822state (esmval- tool.diag_scripts.mlr.models.svr.SVRModel property), 831 L_plot_provenance() (esmval- tool.diag_scripts.monitor.monitor_base.MonitorBase method), 845 cer_mlr_model() (esmval- tool.diag_scripts.mlr.models.gbr_base.GBRModel class method), 710 cer_mlr_model() (esmval- tool.diag_scripts.mlr.models.gbr_sklearn.SklearnGBRModel class method), 727</pre>
<pre>tool.diag_scripts.mlr.models.rfr.RFRModel     method), 806 print_regression_metrics() (esmval- random     tool.diag_scripts.mlr.models.ridge.RidgeModel     method), 814 print_regression_metrics() (esmval- random     tool.diag_scripts.mlr.models.ridge_cv.RidgeCVModel     method), 822 print_regression_metrics() (esmval- random     tool.diag_scripts.mlr.models.svr.SVRModel     method), 831 ProvenanceLogger (class in esmval- random     tool.diag_scripts.shared), 620 Q record quickplot() (in module esmval-     tool.diag_scripts.shared.plot), 633 R random_state (esmval-     tool.diag_scripts.mlr.models.gbr_base.GBRModel     regiss     property), 710 random ctate     (asmval-</pre>	<pre>tool.diag_scripts.mlr.models.MLRModel property), 702state (esmval- tool.diag_scripts.mlr.models.rfr.RFRModel property), 806state (esmval- tool.diag_scripts.mlr.models.ridge_cv.RidgeCVModel property), 814state (esmval- tool.diag_scripts.mlr.models.ridge_cv.RidgeCVModel property), 822state (esmval- tool.diag_scripts.mlr.models.svr.SVRModel property), 831 L_plot_provenance() (esmval- tool.diag_scripts.mlr.models.gbr_base.GBRModel class method), 710 ere_mlr_model() (esmval- tool.diag_scripts.mlr.models.gbr_sklearn.SklearnGBRModel class method), 727 ere_mlr_model() (esmval- tool.diag_scripts.mlr.models.gbr_stlearn.SklearnGBRModel class method), 727 ere_mlr_model() (esmval- tool.diag_scripts.mlr.models.gbr_stlear</pre>
<pre>tool.diag_scripts.mlr.models.rfr.RFRModel     method), 806 print_regression_metrics() (esmval- random     tool.diag_scripts.mlr.models.ridge.RidgeModel     method), 814 print_regression_metrics() (esmval- random     tool.diag_scripts.mlr.models.ridge_cv.RidgeCVModel     method), 822 print_regression_metrics() (esmval- random     tool.diag_scripts.mlr.models.svr.SVRModel     method), 831 ProvenanceLogger (class in esmval- random     tool.diag_scripts.shared), 620 Q record quickplot() (in module esmval-     tool.diag_scripts.shared.plot), 633 R random_state (esmval-     tool.diag_scripts.mlr.models.gbr_base.GBRModel     regiss-     property), 710</pre>	<pre>tool.diag_scripts.mlr.models.MLRModel property), 702state (esmval- tool.diag_scripts.mlr.models.rfr.RFRModel property), 806state (esmval- tool.diag_scripts.mlr.models.ridge_CVModel property), 814state (esmval- tool.diag_scripts.mlr.models.svr.SVRModel property), 822state (esmval- tool.diag_scripts.mlr.models.svr.SVRModel property), 831 L_plot_provenance() (esmval- tool.diag_scripts.monitor.monitor_base.MonitorBase method), 845 cer_mlr_model() (esmval- tool.diag_scripts.mlr.models.gbr_base.GBRModel class method), 710 cer_mlr_model() (esmval- tool.diag_scripts.mlr.models.gbr_sklearn.SklearnGBRModel class method), 727</pre>

<pre>register_mlr_model()</pre>			pipeline()	(esmval-
tool.diag_scripts.mlr.models.gpr_skl	learn.Sklear	nGPRMod	lelool.diag_scripts.mlr.mo	dels.huber.HuberRegressionModel
class method), 748			<i>method</i> ), 756	
<pre>register_mlr_model()</pre>	(esmval-	reset_p	pipeline()	(esmval-
tool.diag_scripts.mlr.models.huber.H	HuberRegres	sionMode	l tool.diag_scripts.mlr.mo	dels.krr.KRRModel
class method), 756			<i>method</i> ), 764	
<pre>register_mlr_model()</pre>	(esmval-	reset_p	pipeline()	(esmval-
tool.diag_scripts.mlr.models.krr.KRI	RModel		tool.diag_scripts.mlr.mo	dels.lasso.LassoModel
class method), 764			method), 772	
<pre>register_mlr_model()</pre>	(esmval-	reset_p	pipeline()	(esmval-
tool.diag_scripts.mlr.models.lasso.L	assoModel		tool.diag_scripts.mlr.mo	dels.lasso_cv.LassoCVModel
class method), 772			method), 781	
<pre>register_mlr_model()</pre>	(esmval-	reset_p	pipeline()	(esmval-
tool.diag_scripts.mlr.models.lasso_c				dels.lasso_lars_cv.LassoLarsCVModel
class method), 780			method), 789	
<pre>register_mlr_model()</pre>	(esmval-	reset_p	pipeline()	(esmval-
tool.diag_scripts.mlr.models.lasso_l				dels.linear.LinearRegressionModel
class method), 789	_		method), 798	0
register_mlr_model()	(esmval-	reset_r	pipeline()	(esmval-
tool.diag_scripts.mlr.models.linear.L				dels.linear base.LinearModel
class method), 798			<i>method</i> ), 718	
register_mlr_model()	(esmval-	reset r	pipeline()	(esmval-
tool.diag_scripts.mlr.models.linear_				
class method), 718	000000000000000000000000000000000000000		method), 702	
register_mlr_model()	(esmval-	reset r	<pre>pipeline()</pre>	(esmval-
tool.diag_scripts.mlr.models.MLRM		10000_1	tool.diag_scripts.mlr.mo	
class method), 702	ouer		method), 806	
register_mlr_model()	(esmval-	reset r	pipeline()	(esmval-
tool.diag_scripts.mlr.models.rfr.RFK		<b>_</b> I	tool.diag_scripts.mlr.mo	×
class method), 806			<i>method</i> ), 814	
register_mlr_model()	(esmval-	reset r	pipeline()	(esmval-
tool.diag_scripts.mlr.models.ridge.R		1 00 0 0_r		dels.ridge_cv.RidgeCVModel
class method), 814	lagemouel		method), 823	acis.ruge_crittuge c rinouer
register_mlr_model()	(esmval-	reset r	<pre>pipeline()</pre>	(esmval-
tool.diag_scripts.mlr.models.ridge_c			tool.diag_scripts.mlr.mo	
class method), 822	viituge e v ii	iouci	method), 831	
register_mlr_model()	(esmval-	rfecv()	<i>,,</i>	mlr.models.gbr_base.GBRModel
tool.diag_scripts.mlr.models.svr.SVF			method), 710	minimodelis.gor_base.obranodel
class method), 831	linouei			mlr.models.gbr_sklearn.SklearnGBRMo
regression_line() (in module	esmval-	11000()	method), 727	minimodelis.gor_skiedi n.skiedi nODKiro
tool.diag_scripts.emergent_constrain		rfacy()		mlr.models.gbr_xgboost.XGBoostGBRM
646		11000()	method), 735	
reset_pipeline()	(esmval_	rfecv()	, · ·	mlr.models.gpr_sklearn.SklearnGPRMo
tool.diag_scripts.mlr.models.gbr_ba			method), 748	mir.models.gpr_sklearn.sklearnOr Kino
method), 710	se.ODRmou			mlr.models.huber.HuberRegressionMod
reset_pipeline()	(esmval-	TIECV	method), 756	mir.models.nuber.muber.regressionwiod
tool.diag_scripts.mlr.models.gbr_skl		n GE BRANK		mlr models krr KPPModel
	eum.skieum		method), 764	mir.models.krr.KKKModel
method), 727	(asmual	mfo.cu()		mlumodolo lasso LassoModol
<pre>reset_pipeline()</pre>				mlr.models.lasso.LassoModel
	00051.AGD0			mlrmodals lasso on Lasso CVM adal
<pre>method), 735 reset_pipeline()</pre>	(esmval-	TTECA	(esmvattool.atag_scripts. method), 781	mlr.models.lasso_cv.LassoCVModel
		n GE P.P.A.A.A.S		mlr.models.lasso_lars_cv.LassoLarsCV
method), 748	ean n. skiedri	I U I DUY (L)	method), 789	minimoueis.iusso_iurs_cv.LussoLursCv1
<i>memou</i> ), <i>i</i> +0			11011001, 107	

#### ESMValTool User's and Developer's Guide, Release 2.11.0.dev52+g696097c.d20240424

<b>rfecv()</b> (esmvaltool.diag_scripts.mlr.models.linear.LinearRe		
		esmval-
<pre>rfecv() (esmvaltool.diag_scripts.mlr.models.linear_base.Lin</pre>	nearModtdol.diag_scripts.mlr.custom_sklearn.Aa method), 680	wancedRFECV
<pre>rfecv() (esmvaltool.diag_scripts.mlr.models.MLRModel s</pre>	set_fit_request() (a	esmval-
<i>method</i> ), 702	tool.diag_scripts.mlr.custom_sklearn.Aa	lvancedTransformedTarge
<b>rfecv()</b> ( <i>esmvaltool.diag_scripts.mlr.models.rfr.RFRModel</i>	<i>method</i> ), 684	
		esmval-
<pre>rfecv() (esmvaltool.diag_scripts.mlr.models.ridge.RidgeMo method), 814</pre>	odel tool.diag_scripts.mlr.custom_sklearn.Aa method), 671	wancedPipeline
<pre>rfecv() (esmvaltool.diag_scripts.mlr.models.ridge_cv.Ridgs</pre>	eV_Mondplut() (6	esmval-
<i>method</i> ), 823	tool.diag_scripts.mlr.custom_sklearn.Aa	lvancedRFE
<pre>rfecv() (esmvaltool.diag_scripts.mlr.models.svr.SVRModel</pre>		
		esmval-
RFRModel (class in esmval- tool.diag_scripts.mlr.models.rfr), 798	tool.diag_scripts.mlr.custom_sklearn.Aa method), 681	wancedRFECV
		esmval-
tool.diag_scripts.mlr.models.ridge_cv), 815 RidgeModel (class in esmval-	tool.diag_scripts.mlr.custom_sklearn.Fe method), 688	atureSelectionTransform
tool.diag_scripts.mlr.models.ridge), 807 s	set_params() (a	esmval-
rounds_sig() (in module esmval-	tool.diag_scripts.mlr.custom_sklearn.Aa	lvancedPipeline
tool.diag_scripts.ocean.diagnostic_model_vs_obs),	, <i>method</i> ), 671	
851 s		esmval-
<pre>run_diagnostic() (in module esmval-</pre>	tool.diag_scripts.mlr.custom_sklearn.Aa	lvancedRFE
tool.diag_scripts.shared), 626	<i>method</i> ), 676	
°, s	-1 0	esmval-
S	tool.diag_scripts.mlr.custom_sklearn.Ad	vancedRFECV
<pre>sample_y() (esmvaltool.diag_scripts.mlr.models.gpr_sklear</pre>	n.AdvancealGaussianProcessRegressor	1
memora), 150	-1 0	esmval-
<pre>save_data() (in module esmval- tool.diag_scripts.shared), 626</pre>	tool.diag_scripts.mlr.custom_sklearn.Aa method), 685	
-		esmval-
tool.diag_scripts.shared), 627 scatterplot() (in module esmval-	tool.diag_scripts.mlr.custom_sklearn.Fe method), 689	atureSelectionTransform
tool.diag_scripts.shared.plot), 633	set_params() (a	esmval-
score() (esmvaltool.diag_scripts.mlr.custom_sklearn.Advan method), 670	method), 739	
score() (esmvaltool.diag_scripts.mlr.custom_sklearn.Advan	etd <b>pro</b> t_appearance() (in module	esmval-
<i>method</i> ), 675	tool.diag_scripts.emergent_constraints),	1
<pre>score() (esmvaltool.diag_scripts.mlr.custom_sklearn.Advan</pre>	ncedRFE@\$6	
		esmval-
<pre>score() (esmvaltool.diag_scripts.mlr.custom_sklearn.Advan method), 683</pre>	method), 677	
<pre>score() (esmvaltool.diag_scripts.mlr.models.gpr_sklearn.A</pre>		esmval-
method), 739	tool.diag_scripts.mlr.custom_sklearn.Aa	vanceaRFECV
<pre>score_samples() (esmval-</pre>	method), 682	esmval-
tool.diag_scripts.mlr.custom_sklearn.AdvancedPip	tool.diag_scripts.mlr.custom_sklearn.Aa	
method), 671	method), 685	vanceurransjormeurarge
<pre>select_metadata() (in module esmval-</pre>		esmval-
ioonanas_senipis.snanea), ozi	tool.diag_scripts.mlr.models.gpr_sklear	
<pre>set_data() (esmvaltool.diag_scripts.shared.Datasets     method), 619</pre>	method), 739	zavanceu Gunssiuni 10
set_fit_request() (esmval- <sup>S</sup>		esmval-
tool.diag_scripts.mlr.custom_sklearn.AdvancedRFI		
or		

<i>method</i> ), 671	<pre>test_normality_of_residuals() (esmval-</pre>
set_score_request() (esmval-	tool.diag_scripts.mlr.models.gbr_xgboost.XGBoostGBRModel
tool.diag_scripts.mlr.custom_sklearn.AdvancedT	
<i>method</i> ), 686	test_normality_of_residuals() (esmval-
<pre>set_score_request() (esmval-</pre>	tool.diag_scripts.mlr.models.gpr_sklearn.SklearnGPRModel
tool.diag_scripts.mlr.models.gpr_sklearn.Advanc	
<pre>method), 740 short_name (esmvaltool.diag_scripts.shared.Variable</pre>	<pre>test_normality_of_residuals() (esmval- tool.diag_scripts.mlr.models.huber.HuberRegressionModel</pre>
attribute), 622	method), 757
	test_normality_of_residuals() (esmval-
tool.diag_scripts.shared.Variables method),	tool.diag_scripts.mlr.models.krr.KRRModel
623	<i>method</i> ), 764
	test_normality_of_residuals() (esmval-
tool.diag_scripts.shared.Variables method),	tool.diag_scripts.mlr.models.lasso.LassoModel
623 SklearnGBRModel (class in esmval-	<pre>method), 773 test_normality_of_residuals() (esmval-</pre>
tool.diag_scripts.mlr.models.gbr_sklearn),	tool.diag_scripts.mlr.models.lasso_cv.LassoCVModel
719	method), 781
SklearnGPRModel (class in esmval-	<pre>test_normality_of_residuals() (esmval-</pre>
tool.diag_scripts.mlr.models.gpr_sklearn),	tool.diag_scripts.mlr.models.lasso_lars_cv.LassoLarsCVModel
741	method), 790
	test_normality_of_residuals() (esmval-
<pre>tool.diag_scripts.shared), 627 sorted_metadata() (in module esmval-</pre>	tool.diag_scripts.mlr.models.linear.LinearRegressionModel method), 798
tool.diag_scripts.shared), 627	test_normality_of_residuals() (esmval-
square_root_metadata() (in module esmval-	tool.diag_scripts.mlr.models.linear_base.LinearModel
tool.diag_scripts.mlr), 663	method), 719
	test_normality_of_residuals() (esmval-
tool.diag_scripts.shared.Variable attribute),	tool.diag_scripts.mlr.models.MLRModel
622 standard_name() (esmval-	method), 702
<pre>standard_name() (esmval- tool.diag_scripts.shared.Variables method),</pre>	<pre>test_normality_of_residuals() (esmval- tool.diag_scripts.mlr.models.rfr.RFRModel</pre>
624	method), 806
	<pre>test_normality_of_residuals() (esmval-</pre>
tool.diag_scripts.shared.Variables method),	tool.diag_scripts.mlr.models.ridge.RidgeModel
624	<i>method</i> ), 815
<pre>standard_prediction_error() (in module esmval-</pre>	
tool.diag_scripts.emergent_constraints), 647 steps (esmvaltool.diag_scripts.mlr.custom_sklearn.Advan	tool.diag_scripts.mlr.models.ridge_cv.RidgeCVModel
attribute), 672	test_normality_of_residuals() (esmval-
SVRModel (class in esmval-	tool.diag_scripts.mlr.models.svr.SVRModel
tool.diag_scripts.mlr.models.svr), 823	method), 831
<b>T</b>	timeplot() (in module esmval-
T	tool.diag_scripts.ocean.diagnostic_timeseries),
target_pdf() (in module esmval-	854
tool.diag_scripts.emergent_constraints),	titlify() (in module esmval- tool.diag_scripts.ocean.diagnostic_transects),
647 test_normality_of_residuals() (esmval-	857
<pre>test_normality_of_residuals() (esmval- tool.diag_scripts.mlr.models.gbr_base.GBRMode</pre>	
method), 710	tool.diag_scripts.mlr.custom_sklearn.AdvancedPipeline
<pre>test_normality_of_residuals() (esmval-</pre>	<i>method</i> ), 672
tool.diag_scripts.mlr.models.gbr_sklearn.Sklearn	(csmval-
<i>method</i> ), 727	tool.diag_scripts.mlr.custom_sklearn.AdvancedRFE
	<i>method</i> ), 677

transfo				parameters()	(esmval-
	tool.diag_scripts.mlr.custom_sklearn. method), 682	AdvancedR.	FECV	tool.diag_scripts.mlr.models.linear_l method), 719	base.LinearModel
transfo	rm()	(esmval-	update_	parameters()	(esmval-
	tool.diag_scripts.mlr.custom_sklearn. method), 689		-	sformdiag_scripts.mlr.models.MLRMa method), 702	
transfo	rm_only()	(esmval-	update_	parameters()	(esmval-
	tool.diag_scripts.mlr.custom_sklearn. method), 673	AdvancedP	ipeline	tool.diag_scripts.mlr.models.rfr.RFR method), 806	Model
	<pre>rm_target_only()</pre>	(esmval-	update_	parameters()	(esmval-
	tool.diag_scripts.mlr.custom_sklearn. method), 673	AdvancedP.		tool.diag_scripts.mlr.models.ridge.Ri method), 815	idgeModel
			update_	parameters()	(esmval-
U				tool.diag_scripts.mlr.models.ridge_cr	v.RidgeCVModel
unify_1	d_cubes() (in module	esmval-		method), 823	
	tool.diag_scripts.shared.iris_helpers)	, 630	update_	parameters()	(esmval-
unify_t:	ime_coord() (in module	esmval-		tool.diag_scripts.mlr.models.svr.SVR	Model
	tool.diag_scripts.shared.iris_helpers)	, 630		<i>method</i> ), 831	
	(esmvaltool.diag_scripts.shared.Varia tribute), 622	able at-	V		
units()	(esmvaltool.diag_scripts.shared method), 624	.Variables	var_nam	<b>ne()</b> (esmvaltool.diag_scripts.sharea method), 624	l.Variables
units_po	ower() (in module	esmval-	Variabl	e (class in esmvaltool.diag_scripts.sh	ared), 621
	tool.diag_scripts.mlr), 663		Variabl	es (class in esmvaltool.diag_scrip.	ts.shared),
update_j	parameters()	(esmval-		622	
	tool.diag_scripts.mlr.models.gbr_bas method), 711	e.GBRMode	wariabl	<pre>es_available() (in module tool.diag_scripts.shared), 628</pre>	esmval-
update_j	parameters()	(esmval-	vars_av	vailable()	(esmval-
	tool.diag_scripts.mlr.models.gbr_skle method), 727	earn.Sklearn	GBRMod	elool.diag_scripts.shared.Variables 624	method),
	parameters()	(esmval-	V		
	tool.diag_scripts.mlr.models.gbr_xgb method), 736	oost.XGBoo		odel GBRModel (class in	esmval-
update_j	parameters()	(esmval-		tool.diag_scripts.mlr.models.gbr_xgl	poost),
	tool.diag_scripts.mlr.models.gpr_skle method), 748	earn.Sklearn	GPRMod		
update_j	parameters()	(esmval-			
	tool.diag_scripts.mlr.models.huber.H method), 757	uberRegress	sionModel	1	
update_j	parameters()	(esmval-			
	tool.diag_scripts.mlr.models.krr.KRR method), 765	Model			
update_j	parameters()	(esmval-			
	tool.diag_scripts.mlr.models.lasso.La method), 773	ussoModel			
update_j	parameters()	(esmval-			
	tool.diag_scripts.mlr.models.lasso_cw method), 781	v.LassoCVM	odel		
	parameters()	(esmval-			
	tool.diag_scripts.mlr.models.lasso_la method), 790	ers_cv.Lasso	LarsCVM	lodel	
	parameters()	(esmval-			
	tool.diag_scripts.mlr.models.linear.Li method), 798		sionMode	l	